SIZE-SENSITIVE CRYSTAL PLASTICITY
FINITE ELEMENT FRAMEWORK FOR
SIMULATING BEHAVIOR OF LAMELLAR
METAL-METAL COMPOSITES

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SIZE-SENSITIVE CRYSTAL PLASTICITY FINITE ELEMENT FRAMEWORK FOR SIMULATING BEHAVIOR OF LAMELLAR METAL-METAL COMPOSITES

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Submitted to the University of New Hampshire in Partial Fulfillment of the Requirements for the Degree of

Doctor of Philosophy
in
Mechanical Engineering

December, 2017
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DEDICATION

I would like to dedicate my dissertation work to the love of my life, my wife Jovana. Without your immense support, love and understanding this whole journey would just not be the same. I would also like to express a special feeling of gratitude to my family, to my loving parents, Ivanka and Petar, whose encouragements motivated me to pursue my dreams, and to my dear sister Marija, who has always been there for me to cheer me and be my biggest supporter.
ACKNOWLEDGEMENTS

I would like first to thank my academic advisor, Professor Marko Knezevic, for his continuous and unlimited support throughout my PhD program.

I would also like to express my sincere gratitude to the rest of my dissertation committee: Prof. Irene Beyerlein, Prof. Todd Gross, Prof. Ioannis Korkolis, Prof. Igor Tsukrov and Prof. Mark Lyon. Your insightful comments and suggestions, as well as challenging questions motivated me to push my limits to the edge of possible and they advanced my research. I would particularly like to thank Prof. Irene Beyerlein, who provided me with an opportunity to work with her at Los Alamos National Laboratory. It was my great pleasure and honor.

Furthermore, I would like to acknowledge the support from the Graduate School at the University of New Hampshire provided through Dissertation Year Fellowship program.

My gratitude also goes to my officemates from S225, and the rest of my colleagues and friends, who all unconditionally supported me in this endeavor.
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ABSTRACT

SIZE-SENSITIVE CRYSTAL PLASTICITY FINITE ELEMENT FRAMEWORK FOR SIMULATING BEHAVIOR OF LAMELLAR METAL-METAL COMPOSITES

by

Milan Ardeljan

University of New Hampshire, December, 2017

Growing demands for materials with enhanced and superb characteristics increase the difficulty and the amount of research necessary to be conducted in many different areas of expertise. The vast field of computational mechanics represents a significant source of valuable solutions to many of these challenges and can provide a smoother transition in the process when a new material is introduced. Experimental techniques are not always able to measure the localized material features due to the very complicated deformation conditions. As an alternative approach, full-field models are developed, such as the ones contained in this dissertation that can bridge this gap and provide source of significant insights. The crystal plasticity finite element models (CPFEM) developed under this dissertation are presented and discussed through several specific case studies, which establish the fundamental microstructure-property relationships that describe in particular the deformation behavior of novel multilayer metallic lamellar microstructures composed of Zirconium-Niobium and Magnesium-Niobium layers. These lamellar material systems exhibit extraordinary strength while preserving ductility and they are promising candidates for application in many industries, such as nuclear and automotive. Different formulations of the 3D multiscale models were numerically implemented to investigate the origin and the development of the microstructural features that occurred during the fabrication process of these lamellar composites. In particular, the orientation stability of nanocrystalline Zirconium and the formation of strain localizations were investigated during accumulative roll bonding process. Furthermore, the work contained in this dissertation describes the first attempt to incorporate the confined layer slip (CLS) model into CPFEM, which greatly contributes to fundamental understanding of how Magnesium-Niobium nano-layered composites deform elastically and plastically at nanometer length scales. Next, significant efforts were put into investigating a mechanism of deformation twinning. This deformation mechanism governs the mechanical behavior of many polycrystalline metals, particularly those with low symmetry crystal structures. Deformation twins are represented as lamellar inclusions in the granular microstructures, and overall the material behaves as a composite. Hence, a novel modeling approach, which explicitly models the formation and thickening of a twin lamella within a crystal plasticity finite element framework was developed. The model represents a unique numerical procedure which is able to relate spatially resolved fields of stress and strains with microstructural changes during a twin formation and thickening. This approach was applied to
study the twin formation and thickening in cast Uranium and Magnesium alloy AZ31. In AZ31 the effects of dislocation density on a twin propagation were investigated, as well as the influence of the double twin formation on the material’s fracture behavior. Overall, the presented work in my dissertation provides a powerful predictive simulation tool that could be used in many subsequent studies contributing to the further advancements in the field of computational material science.
INTRODUCTION

The field of material science is immense and very diverse. Chronologically, the emergence of specific materials gave name to the particular historical ages that produced some of the most advanced civilizations of the time. One of the hallmarks of the modern industrialized societies is our increasing need to use different materials. We use more materials than ever before and we also deplete them at even faster rates. Hence, the development of new materials is ever-present demand, which makes it a challenge for the generations to come. This demand is becoming very vital with ever growing demand for energy efficient and sustainable designs in many engineering-related fields. Also, enlarged consumption of materials means that we need to find better ways to employ existing raw materials more efficiently, to recycle waste materials and make them reusable, and to produce brand new materials out of substances which are abundantly available in the nature.

These new materials, developed for many specific industrial applications, provide better design performance, and they are proven to be more advantageous in comparison to classical materials. Therefore, a formidable amount of research is necessary to be conducted in many different areas of expertise encompassing both experimental and modelling techniques. In order to fully understand how materials mechanically behave they need to be investigated at different length scales. The major goal of the presented work in this dissertation is to analyze and understand the fundamental phenomenological mechanisms that govern deformation of such novel materials. An approach that enables this and that has been widely used takes into consideration developing of novel crystal plasticity finite element models (CPFEM). The models represent a valuable asset and provide simulation capability, which can enable us to investigate mechanical behavior of materials in terms of various microstructural features. In the vast field of
computational material science, it is believed that this type of approach can help in the development of new materials by reducing the number of trials and errors in the classical experimental procedures. The efforts and results presented in this dissertation are contribution in this direction.

My dissertation is manuscript-based and consists of several integral parts. More specifically, there are 8 chapters with each chapter representing an individual research study presented in a form of a manuscript/research article. A brief summary of each chapter is given next, highlighting the significance and novelty of each study. In all of them, crystal plasticity finite element framework was used to simulate and predict mechanical response of different materials that were studied.

In chapter 1, T-CPFE, a multi-level model for polycrystalline metals that deform by slip and deformation twinning is developed. The macro-level model employs finite element homogenization, whereas the meso-level model uses a Taylor-type model. The meso-level model integrates a new twinning model for handling multiple twin variants per grain. The particular methodology for twinning is the total Lagrangian numerical scheme combined with the advanced composite grain twinning model. The grain level model features a dislocation density based hardening law. The model is applied to magnesium alloy AZ31 and it is calibrated and validated on a comprehensive experimental data set collected in compression, tension, and torsion for extruded AZ31 alloy over temperature ranging from 77 K to 423 K and strain rates ranging from $10^{-4}$ s$^{-1}$ to 3000 s$^{-1}$. This is the first succesful application to hexagonal metal of a Taylor-type model and finite element combination wherein the iso-strain assumption intrinsic to Taylor was relaxed.
Chapter 2 presents a 3D multiscale model for polycrystalline metals. The model uniquely incorporates a dislocation density-based hardening law for multiple slip modes into a single-crystal plasticity model, which in turn is linked to the polycrystalline response using finite elements. The model is applied to the challenging problem of a bi-phase Zr/Nb layered composite that is deformed to large strains. Both Zr and Nb are known to deform by multiple slip modes in monolithic form. The model predictions indicate that for the Zr phase within the composite, prismatic slip is predominant, yet some amount of pyramidal and basal slip activate in the later stages of deformation. In the Nb phase, both {110} and {112} slips are active, with the former providing more accommodation. This is a unique polycrystal model which is able to connect spatially resolved fields of dislocations, stress, strain, and lattice reorientation with microstructural features such as grain (homophase) and bimetal (heterophase) boundaries.

Chapter 3 describes a developed 3D microstructure based, multi-scale crystal plasticity finite element (CPFE) model. It is applied to understand the relationship between microstructure and strain localizations during plane strain compression of a two-phase hexagonal closed-packed/body-centered cubic (HCP/BCC) Zr/Nb lamellar composite. Experimentally informed representations of the deformed or annealed polycrystalline grain structures within Zr/Nb micron-layered composites were constructed in DREAM.3D. A meshing toolset was then developed to mesh the grains and grain boundary network within these DREAM.3D microstructure models. The constitutive model used a dislocation density based hardening law, wherein the dislocation densities for the multiple modes of slip in Zr and Nb evolve with their own individual dependencies on strain, temperature, and strain rate. With this multiscale modeling approach and DREAM.3D microstructural representations of grain topology, the microstructure is better linked with the strain localizations that can precede the development of
shear bands. The studies provide insight into the relationship between grain structure and the onset of strain localization.

In chapter 4, the already developed 3D multiscale CPFE model (described in chapters 2 and 3) was used to study the orientational stability of nanocrystalline Zr in rolling. The studied material is again nano-layered Zr/Nb composites. It was reported that once the layers reduce below 100 nm, the texture became unusually highly oriented in a few special orientations. Thus, the nanolayered Zr phase provided the opportunity to study potentially unconventional aspects of plastic deformation of nanocrystalline hcp Zr, as well as the effects of co-deformation between the Zr/Nb nanocrystals.

Chapter 5 presents a combination of experiment and computational techniques that were used to gain insight into the deformation mechanisms underlying the room temperature deformation of the BCC Mg phase in nanolayered composites. Both multilayered 5/5 nm BCC Mg/ BCC Nb (5 nm BCC Mg) and 50/50 nm HCP Mg/ BCC Nb (50 nm HCP Mg) composites were fabricated via physical vapor deposition and tested via micropilar compression. A crystal plasticity finite element model was built to simulate the compression deformation of the pillar. The model newly introduced confined layer slip (CLS) for dislocation glide resistance at the slip system level in place of the conventional layer size-independent dislocation density hardening law.

Chapter 6 shows a novel approach for modeling deformation twinning by explicit incorporation of twin lamellae into a 3D crystal plasticity finite element framework. The presented approach accounts for both the morphological and crystallographic reorientation associated with the formation and thickening of a twin lamella. The framework is applied to uranium, a material with an orthorhombic crystal structure. The CPFE model is modified for the first time to include the shear transformation strain associated with deformation twinning. The
effects of the microstructural characteristics such as grain structure and grain boundaries are explicitly modeled.

In chapter 7, following the work presented in the previous chapter, the already developed framework was used to investigate the effects of dislocation density on twin propagation. For a magnesium alloy AZ31 containing extension twins, we calculated the stress fields and analyzed the driving forces for twin growth for three cases of twin dislocation density: full recovery (the twin domain removes the stored dislocation density and sets them to their initial values), maintenance (the twin domain retains it), and the Basinski effect (the twin domain adopts a much larger stored dislocation density, by two times in this case). In the modeling approach, the twin is thickened according to a criterion that maintains the stress state in the vicinity of the grain at a pre-defined characteristic twin resistance. The calculations show that most of the averaged properties, such as the rate of dislocation storage in the entire twin grain, the twin growth rate, the stress field in the twinned grain and neighboring grains, and the slip activity in the parent matrix are not significantly altered by dislocation storage in the twin.

Finally, in chapter 8, the same CPFE framework already mentioned in the previous two chapters was extended to model a discrete double twin lamella. A number of studies have found that the formation of double twins in low symmetry metals can lead to the onset of strain localizations, leading further to void nucleation and ultimately fracture. Hence, this novel study is again applied to magnesium alloy AZ31. The simulations predict that the distribution of local stress-strain fields during formation and growth of primary contraction twin causes the formation of a secondary extension twin variant, which is consistent with experimental observations in both compression and tension. The primary contraction twin region was predicted to deform by a large amount of basal slip. The investigation of the traction forces acting on a double twin-parent
interface revealed that the contraction twin-parent interface is a weak link in the microstructural grain boundary network, which is susceptible to void nucleation.
Chapter 1

This chapter was published as: Strain rate and temperature sensitive multi-level crystal plasticity model for large plastic deformation behavior: Application to AZ31 magnesium alloy, Milan Ardeljan, Irene J. Beyerlein, Brandon A. McWilliams, Marko Knezevic, International Journal of Plasticity, 83, 90-109. My role in preparing this chapter was to numerically implement the developed crystal plasticity finite element model, which describes the material large plastic deformation, and to successfully apply it to magnesium alloy AZ31. The model was calibrated against a comprehensive experimental data set that consisted of measured material stress-strain responses and deformed textures that corresponded to different deformation modes at various temperatures and strain rates. I was in charge of performing the modeling study and post-processing of all the data necessary to create figures and graphs that are shown in this chapter. Furthermore, I contributed in the process of composing the paper by writing the sections relevant to the modeling work that was performed.
Strain rate and temperature sensitive multi-level crystal plasticity model for large plastic deformation behavior: Application to AZ31 magnesium alloy

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Abstract

In this work, we develop a multi-level constitutive model for polycrystalline metals that deform by a combination of elasticity, slip and deformation twinning. It involves a two-level homogenization scheme, where the first level uses an upper bound Taylor-type crystal plasticity (T-CP) theory to relate the single-crystal scale to the polycrystal meso-scale and the second level employs an implicit finite elements (FE) approach to relate the meso-scale to the macro-scale. The latter relaxes the iso-strain constraints imposed by the Taylor model. As such, we name the model T-CPFE. At the single crystal level, the model features a dislocation-based hardening law providing the activation stresses that governs slip activity within the single crystals. For deformation twinning, it contains an advancement of a composite grain model that retains the total Lagrangian formulation. Here we use the T-CPFE model to analyze the mechanical response and microstructure evolution of extruded AZ31 Mg alloy samples in simple compression, tension, and torsion under strain rates ranging from $10^{-4}$ s\textsuperscript{-1} to 3000 s\textsuperscript{-1} and temperatures ranging from 77 K to 423 K reported in (Kabirian et al., 2015). Taking the experimentally measured initial texture and average grain size as inputs, the model successfully captures stress-strain responses, deformation texture evolution and twin volume fraction using a single set of material parameters associated with the thermally activated rate laws for dislocation density. The distinctions in flow stress evolution among the loading conditions result from
differing relative amounts of slip and twinning activity, which the model internally adjusts based on evolution of slip and twin resistances in the response to the imposed loading conditions. Finally, we show that the T-CPFE model predictions of geometrical changes during compression compare favorably with corresponding geometry of samples deformed experimentally. For this application, it predicts the anisotropy and asymmetry of the material flow resulting from crystallographically soft-to-deform extension twinning and basal slip and hard-to-deform contraction twinning and pyramidal slip. The formulation developed is sufficiently general that the T-CPFE model can be applied to other materials that slip and twin.

*Keywords:* A. Microstructures; A. Twinning; B. Crystal plasticity; B. Anisotropic material; C. Finite elements; T-CPFE UMAT

1. **Introduction**

The constitutive response of polycrystalline metals is a result of the collective deformation responses of its many constituent grains having different crystal orientation, shape, and size (Kocks et al., 1998). For metallic crystals with a hexagonal closed packed (HCP) structure, the deformation behavior is highly anisotropic, both elastically and plastically (Akhtar, 1973; Partridge, 1967; Yoo, 1981). The latter can be carried by both slip and deformation twinning on multiple systems, differing in crystallography and activation stresses and exhibiting differing dependencies on temperature and strain rate (Akhtar, 1975; Akhtar and Teghtsoonian, 1969a). As a result, polycrystalline HCP metals and their alloys generally exhibit strong plastic anisotropy and sensitivities to strain rate and temperature (Ishikawa et al., 2005; Khan et al., 2011; Watanabe and Ishikawa, 2009).

Over the years, the constitutive response of HCP metals and their alloys have been modeled using crystal plasticity based techniques. The relationship between the deformation of the crystal
and that of the aggregate has been calculated using mean-field and spatially resolved crystal plasticity mechanics tools. The advantage of the former class over the latter is that computational speeds are substantially greater, large strain deformations have been easier to treat, and its implementation is simpler. These advantages arise from the fact that these methods homogenize the surroundings of each grain (Carpenter et al., 2015; Fromm et al., 2009; Kalidindi, 1998; Knezevic et al., 2013b; Knezevic et al., 2008a; Knezevic and Landry, 2015; Lebensohn and Tomé, 1993; Lentz et al., 2015a; Lentz et al., 2015b; Van Houtte, 1988; Wu et al., 2007a). The latter spatially resolved mechanics tools do not make such assumptions but account for grain-to-grain interactions and therefore have far more flexibility in calculating inhomogeneous mechanical fields, such as those resulting from non-uniform boundary conditions or complicated grain structures or multi-phase materials (Abdolvand et al., 2015; Fernández et al., 2013; Jahedi et al., 2015; Jahedi et al., 2014; Keshavarz and Ghosh, 2015; Knezevic et al., 2014d; Lebensohn et al., 2012; Staroselsky and Anand, 2003). Because both crystal plasticity based techniques are relevant to the present work, they are further discussed below.

1.1 Mean-field techniques

For metals that deform by slip and twinning, mean-field techniques are being used overwhelmingly more often than spatially resolved techniques because of the difficulties with performing spatial grain reorientations due to twinning. Commonly used ones include Taylor-type (Knezevic et al., 2009; Taylor, 1938; Van Houtte, 1988) and self-consistent (SC) (Eshelby, 1957; Lebensohn and Tomé, 1993; Lebensohn et al., 2007) schemes. The latter is the widely used visco-plastic self-consistent (VPSC) model. In the Taylor model, an applied strain in the form of a deformation or velocity gradient over a polycrystal is assumed to be the same in every grain. Since interactions between the constituent grains are not modeled, the Taylor model is
suitable for computationally efficient highly parallelized implementations (Knezevic and Savage, 2014; Mihaila et al., 2014; Sarma et al., 1998; Savage and Knezevic, 2015). In contrast, with SC schemes, individual grains interact with the average response of the polycrystal. This interaction introduces several SC numerical iterations, which make it less suitable for parallelization. A key advantage of mean-field techniques is the ability to capture the influence of the reorientation and shear provided by twin phases within individual grains. To this end, several micromechanical approaches for twinning have been developed. These are the predominant twin reorientation method (Tomé et al., 1991; Van Houtte, 1978), total Lagrangian approach (Fast et al., 2008; Kalidindi, 1998; Wu et al., 2007a), and composite-grain model (Proust et al., 2007).

A benefit of such mean-field polycrystal models is that they can predict the active slip and twinning systems and their relative contributions in each crystal and at each moment in time or at strain level. The relative activity of slip and twinning is responsible for the evolution of texture, plastic anisotropy in flow stress, and hardening behavior. Obtaining the same microscopic information on slip and twinning activity via experiment is challenging. However, such predictions rely on having a reliable set of hardening parameters as input into the mean-field/micromechanical twin scheme. These are best found by identifying a single set of parameters that can capture a large suite of stress-strain, microstructural and texture evolution data obtained from distinctly different mechanical tests (e.g., distinct loading orientations, temperature, strain rate, strain path changes). However, differences in the homogenization scheme, twin-reorientation scheme, and hardening laws can lead to variations in the characterized material parameters for the activation of slip and twinning, even for the same material and the same suite of experimental data.
1.2 Spatial crystal plasticity techniques

The other class of CP constitutive models are spatially resolved crystal plasticity mechanics techniques, such as crystallographic formulations based either on finite element (Abdolvand et al., 2015; Fernández et al., 2013; Kalidindi et al., 2004; Kalidindi et al., 2006; Knezevic et al., 2014c; Zhao et al., 2008) solvers, like crystal plasticity finite element (CPFE), or on Green’s function fast Fourier transform (Lebensohn et al., 2012) solvers, such as the crystal plasticity fast Fourier transform (CP-FFT) model. These techniques can calculate spatially resolved mechanical fields within deformed microstructures, thereby overcoming the local stress state limitations of mean field polycrystalline plasticity techniques. They account for grain-to-grain interactions and predict gradients in strains, orientations, and stresses across grains and grain boundaries. Traditionally, in these methods, the deformation at each point in the material is governed by elasticity, plasticity, and twinning. The material point can lie within a single crystal (Ardeljan et al., 2014; Ardeljan et al., 2015a; Diard et al., 2005; Fernández et al., 2013; Kalidindi et al., 1992; Staroselsky and Anand, 1998, 2003) or represent a polycrystal whose response is obtained by a homogenization scheme, such as Taylor (Zecevic et al., 2015b, c) or VPSC (Knezevic et al., 2016; Knezevic et al., 2014d; Knezevic et al., 2013c). In either case, activation of slip is provided by a separate hardening model, which has varied from a constant critical resolved shear stress (CRSS) model, a phenomenological hardening model (e.g., the Voce or sinh expressions) (Tomé et al., 1984; Voce, 1948), or a dislocation density based hardening model with or without GNDs (Beyerlein and Tomé, 2008; Knezevic et al., 2013a; Zecevic and Knezevic, 2015). These slip resistance models assume that slip occurs homogeneously, whether within a grain in the polycrystal or at every material point, and therefore, they best apply to microstructures containing grains that are two to three orders of magnitude greater in diameter than the
dislocation core size. This inherent assumption has generally limited use of CPFE models for ultra-fine grained and nano-grained materials, although it should be mentioned that a few recent CPFE developments have attempt to overcome this limitation (Li et al., 2009; Yuan et al., 2015).

Last, in these spatially resolved CP models, deformation twinning is typically represented by a pseudo-slip model (Kalidindi, 1998; Van Houtte, 1978). Modeling twins as discrete domains within which the lattice has reoriented and sheared in spatially resolved techniques, such as CPFE and CP-FFT, have been developed only recently (Ardeljan et al., 2015b; Arul Kumar et al., 2015). However, they have yet to be advanced to model in a physically consistent way the formation, propagation, and expansion of a twin domain (Knezevic et al., 2015a).

1.3 Objectives

In this article, we develop a two-level constitutive model that combines a full-field spatially resolved mechanics technique at one level with a mean-field technique at a finer level. The full-field model is built upon a CPFE code, within which spatially resolved stress-strain can be calculated. The mean-field model is the Taylor type model (Wu et al., 2007a) originally developed for α-Ti and, thus, capable of handling crystallographic slip and deformation twinning. We refer to the combined, two-level model as T-CPFE. Here in the T-CPFE model, we introduce further extensions by implementing a more advanced twinning model, called the composite grain (CG) formulation (Proust et al., 2007), while retaining the total Lagrangian numerical scheme. As another advancement, we allow multiple twins to form per grain. For activation of slip within the individual crystals, we employ a recently developed dislocation density (DD) hardening law. The DD law has physically based material parameters associated with the thermally activated rate laws for the evolution of dislocation density (Beyerlein and
Tomé, 2008), such as a friction stress, a drag stress, and the activation barrier for dynamic recovery.

The T-CPFE model relaxes the iso-strain constraint imposed by the Taylor model over the entire polycrystalline aggregate by splitting the polycrystal over a number of finite elements and associated integration points. The finite element method as the field solver interrogates the polycrystal at every integration point with a deformation gradient that varies spatially and therefore relaxes the iso-strain constraint typical to Taylor-type models. Note that the T-CPFE is not relaxing the iso-strain constraint imposed by the Taylor model over a sub-polycrystal embedded at an integration point within finite elements but is relaxing the constraint at the level of the overall polycrystalline material spanning over every FE integration point of the entire FE model. Therefore the overall model consists of many Taylor-type models running within FE integration points. The overall strain imposed over the FE model varies spatially and thus removes the iso-strain constraint over the entire polycrystal but not within a sub-polycrystal embedded at an integration point. As a result, the T-CPFE model can simulate geometrical changes (e.g. geometrical changes of the specimen due to material’s anisotropy), which is an advantage over mean-field homogenization models.

It should be noted that the T-CPFE approach developed here is similar to the FE-VPSC approach since both embed a subpolycrystal at every integration point. The T-CPFE model uses the Taylor-type homogenization while the FE-VPSC model uses the self-consistent formalism of average interactions between individual grains and the homogeneous effective medium at every integration point. The FE-VPSC model can be run with several grain-effective medium linearization procedures such as the affine and $n^{\text{eff}} = 10$ interaction schemes (Tome and Lebensohn, 2011). These two linearization procedures are intermediate approximations that give
responses of a polycrystalline material in-between the Taylor upper bound model (Taylor, 1938) and the Sachs lower bound model (Sachs, 1929). The FE-VPSC model can be further run with either average or individual grain shape evolution options, which is necessary to capture the response of elongated morphology microstructures (Smith et al., 2016). The self-consistent iterations and in particular calculations for the grain shape evolution make the FE-VPSC run slower than T-CPFE. As a result, the number of grains that can be embedded at an integration point in FE-VPSC is generally less than in T-CPFE since the computational time scales linearly with the number of grains. As another drawback, the FE-VPSC formulation works with the relatively low values of the rate sensitivity parameter compared to the T-CPFE model. Computational time scales inversely with the value of the rate sensitivity exponent. While the T-CPFE model can work with the relatively low rate sensitivity exponents, the value that must be set in the FE-VPSC models is high and usually $m=0.125$ for the currently available formulation in the literature (Knezevic et al., 2013c, 2013d, Segurado et al., 2012). Finally the T-CPFE has no limitations in terms of handling multiple twin variants.

The constitutive model developed here is multi-level in nature, in which the above modeling components, ranging from the sub-crystalline scale to the scale of the sample, operate concurrently. For demonstration, we apply the model for predicting strain rate and temperature sensitive response and microstructure evolution of AZ31 Mg alloy to large plastic strains. This is the first successful application to hexagonal metals of a Taylor-type model and finite element combination wherein the iso-strain assumption intrinsic to Taylor has been relaxed. The model achieves good agreement with measurements of the stress-strain response, texture evolution, and twin volume fraction. In all cases, the predictions indicate that the deformation is accommodated by a combination of multiple slip modes and deformation twinning. The differences in flow
stress evolution, however, result from differing relative amounts of slip mode and twinning activity. Apart from the new model development, another main contribution of this work is a complete material parameter set for the DD-based hardening law for the AZ31 Mg alloy material. Last, for validation, the T-CPFE model was used to simulate the geometrical changes of AZ31 cylinders cut in two perpendicular directions and deformed in simple compression. This is the added capability of the model when it operates within finite element frameworks. Predicted geometries were directly compared with photographs of the experimentally deformed cylinders. The results show an excellent agreement.

2. Modeling methodology

Figure 1 shows a schematic of the linked multi-level modelling strategy developed here, the T-CPFE. All these components operate concurrently. At the highest length scale is the FE model of the sample (frame a), which consists of a finite element mesh with integration points (frame b). The constitutive response at each integration point is a cluster of grains (frame c). The relation between the deformation of the grain and that of the cluster is calculated using a Taylor polycrystal model (frame c), where the individual grain response is governed by crystallographic slip and deformation twinning (frame d). The plastic part of grain deformation is governed by crystal plasticity, a theory that relates the plasticity to the underlining activity of the slip and twinning systems. A predominant twin orientation scheme is used to model the lattice re-orientation caused by a particular twin variant when it becomes active to a certain extent. Separate hardening laws are used to define the critical activation stresses for slip and twinning (frame d). The new aspects of this model are the connection across the individual components and a total Lagrangian way of handling twinning, which involves the more advanced composite grain model (Proust et al., 2007). Additionally, this new twinning model can consider multiple
twin variants per grain, within the Taylor polycrystal operating at each FE integration point. 
Since the specific parts of the model are not new, they are briefly reviewed below with the 
particular application of interest, the AZ31 Mg alloy, in mind.

Figure 1 A linked single-crystal to polycrystal to FE macro-scale modeling framework for 
plastic deformation of polycrystals.

2.1 FE – macro-scale 

T-CPFE is a User MATerial (UMAT) subroutine in ABAQUS Standard (2013) and each FE 
integration point in an FE mesh is associated with a set of orientations representing a 
polycrystalline material. While the overall response of the polycrystalline material is obtained by 
the finite element homogenization the meso-scale mechanical response is obtained using the 
Taylor-type homogenization. The overall FE homogenization satisfies both equilibrium and 
compatibility conditions in the weak numerical sense while the nature of the Taylor model is 
such that it locally satisfies only the compatibility conditions between grains. The applied load is 
divided into increments, and the equilibrium at each increment is obtained by means of the FE
analysis in an iterative fashion using a global nonlinear solver. The finite element governing equation ensuring stress equilibrium and strain compatibility in its linearized form is:

\[
\left( \int_V \bar{B}^T J \bar{B} dV \right) \Delta \mathbf{U} = \mathbf{f} - \int_V \bar{B}^T \bar{\sigma} dV,
\]

where \( \bar{B} \) is the strain-displacement matrix, \( J \) is the material Jacobian matrix, \( \Delta \mathbf{U} \) is a displacement increment solution vector, \( \bar{\sigma} \) is the volume average Cauchy stress tensor over constituent grains, and \( \mathbf{f} \) is an applied force vector (Bathe, 1996). Based on imposed boundary conditions over an FE model, the FE code supplies a deformation gradient, \( \mathbf{F} \), and the current time \( t + \Delta t \) into the UMAT subroutine for each integration point along with the previous increment solution filed in terms of the Cauchy stress, \( \sigma^t \), for each crystal orientation, and the set of internal state variables including texture and dislocation density per slip system for each crystal orientation. The user material model provides the volume average Cauchy stresses, \( \bar{\sigma} \), the volume average Jacobian, \( \bar{J} \), and updated material state variables for each integration point at each trial time increment. When convergence in stress equilibrium is achieved by the global nonlinear scheme the current solution (at \( t + \Delta t \) for \( \bar{\sigma} \), and the internal variables are accepted. At this point, the calculation advances to the next strain increment.

2.2 Taylor model – meso-scale

The material at every integration point is a grain cluster of \( K \) grains. A Taylor polycrystal model is used to relate the constitutive response of the grain cluster to the deformation of each of its \( K \) constituent grains (Kalidindi et al., 1992). The average value of the Cauchy stress is obtained using:

\[
\bar{\sigma} = \sum_{k=1}^{K} \varphi_k \sigma_k.
\]

where \( K \) is the total number of distinct orientations, involving both parent grains and child twins. This homogenization scheme satisfies compatibility because the same deformation gradient, \( \mathbf{F} \), is applied to all parent grains and child twins at each integration point but it violates stress
equilibrium between these grains and twins. The Taylor model takes in as input a set of weighted crystal orientations, the slip and twinning systems specific to the material, and a set of hardening constants for the selected slip and twinning hardening laws and provides to the FE calculated average stress response and the Jacobian matrix (Eq. 1). The major advantage of the Taylor model over mean-field models is computational efficiency (Al-Harbi et al., 2010; Bhattacharyya et al., 2015; Duvvuru et al., 2007; Fast et al., 2008; Knezevic and Kalidindi, 2007; Knezevic et al., 2008b; Shaffer et al., 2010; Wu et al., 2007b). The specific version extended here is the elastic, visco-plasticity Taylor model originally developed for α-Ti (Wu et al., 2007a).

2.3 Single crystal response – grain-scale

In this section, we describe the material constitutive model used to relate Cauchy stress to its work conjugate strain at each integration point within each FE in the FE mesh. In describing the material constitutive model, we use the standard continuum mechanics notation when possible where tensors are indicated by boldface symbols and scalars are italicized.

2.3.1 Kinematics of slip and twinning

In what follows, we use superscripts $s$ for slip systems and superscript $\alpha$ for the slip modes to which $s$ belong. Likewise, $\beta$ is used to denote the twin modes to which the twin variant $t$ belongs. The total velocity gradient tensor, $\mathbf{L}$, is additively decomposed into the elastic $\mathbf{L}^e$ and the plastic velocity gradients $\mathbf{L}^p$. The $\mathbf{L}^p$ is further additive decomposed into contributions from slip and twinning as:

$$\mathbf{L}^p = \mathbf{L}^{sl} + \mathbf{L}^{tw},$$  \hspace{1cm} (3)

where $\mathbf{L}^{sl}$ is the velocity gradient due to slip, given by

$$\mathbf{L}^{sl} = \sum_{s}^{N^{sl}} \dot{\gamma} \mathbf{b}_s^{\perp} \otimes \mathbf{n}_s^{\perp},$$  \hspace{1cm} (4a)

and $\mathbf{L}^{tw}$ is the velocity gradient due to twinning, which is,
\[ L^{tw} = \sum_{t}^{N^{tw}} \dot{f}^t S^t b_0^t \otimes n_0^t. \] (4b)

In Eq. (4a), \( \dot{\gamma}^s \) is the shearing rate on slip system \( s \), \( S^t \) is the characteristic twin shear on twin system \( t \), and \( N^{sl} \) and \( N^{tw} \) are respectively the total number of available slip and twin systems. The rate \( \dot{f}^t \) is the rate of change of the twin volume fraction per twin system \( t \). We use a subscript \( o \) to remind of the total Lagrangian scheme meaning that these tensors are always defined in their initial crystal orientation. Hence, \( b_0^s/b_0^t \) and \( n_0^s/n_0^t \) are time independent orthonormal unit vectors representing the slip/twin direction and slip/twin plane normal in a fixed reference configuration, respectively.

Unlike \( L \), which is additively decomposed, the total deformation gradient tensor, \( F \), is multiplicatively decomposed into its elastic and plastic components via:

\[ F = F^e F^p, \] (5)

where \( F^e \) is the deformation gradients due to elastic stretching and lattice rotation and \( F^p \) is the deformation gradient due to plastic deformation. The rate of change of \( F^p \) is given by the following flow rule:

\[ \dot{F}^p = L^p F^p. \] (6)

After integration from \( t \) to \( \tau = t + \Delta t \), it becomes:

\[ F^p(\tau) = \exp(L^p \Delta t) F^p(t). \] (7)

Finally, the exponential is conveniently approximated as:

\[ F^p(\tau) = \{I + \Delta t (L^{sl} + L^{tw})\} F^p(t), \] (8)

where \( I \) is the identity matrix.

The pair of work conjugated stress-strain measures is given by the following constitutive relationship in each crystal:

\[ T^e = CE^e, \quad T^e = F^{-1} \{ (det F^e) \sigma \} F^{-T}, \quad E^e = \frac{1}{2} \{ F^e T F^e - I \}. \] (9)
where $\mathbf{C}$ is the fourth-order elasticity tensor, $\mathbf{T}^e$ is the second Piola-Kirchhoff stress, which is the work conjugate of the Lagrangian finite strain $\mathbf{E}^e$. The elastic stiffness is calculated based on the single crystal elastic constants for Mg: $C_{11} = 0.6395 - 1.43\times10^{-4}T$, $C_{12} = 0.2599 - 1.09\times10^{-5}T$, $C_{13} = 0.2174 - 8.2\times10^{-6}T$, $C_{33} = 0.6708 - 1.74\times10^{-4}T$, $C_{44} = 0.1868 - 7.05\times10^{-5}T$ (Slutsky and Garland, 1957) for each crystal orientation (Landry and Knezevic, 2015; Wu et al., 2007b). To calculate stress, we need to evaluate $\mathbf{F}^e = \mathbf{F}\mathbf{F}^{-1}$, which amounts to calculating:

$$\mathbf{F}\mathbf{P}^{-1}(\tau) \cong \mathbf{F}\mathbf{P}^{-1}(t)\{\mathbf{I} - \Delta t(\mathbf{L}^s + \mathbf{L}^t)\}.$$  \hspace{2cm} (10)

2.3.2 Hardening law for slip

Equation (4) defines the relationship between the shear rates on the slip and twinning systems to the plastic contribution to the strain in the grain. To calculate the shear strain rate, $\dot{\gamma}^s$, for each slip system $s$, we can relate the resolved shear stress, $\tau^s = \mathbf{T}^e \cdot \mathbf{m}_0^s$, on the system to the characteristic resistance $\tau_c^s$ for slip systems according to the following power-law relationship (Asaro and Needleman, 1985; Hutchinson, 1976; Kalidindi, 1998):

$$\dot{\gamma}^s = \dot{\gamma}_0 \left( \frac{\tau^s}{\tau_c^s} \right)^{\frac{1}{m}} \text{sign}(\tau^s),$$  \hspace{2cm} (11)

where $\dot{\gamma}_0$ is a reference slip rate (arbitrarily taken here as $0.001 \text{ s}^{-1}$) and $m$ is the strain rate sensitivity factor (taken here to be 0.01). The low value of $m$ is taken to ensure that the rate sensitivity effects will be governed by the hardening law for the evolution of slip resistance and not from the power law form of the flow rule (Eq. 11). $\mathbf{m}_0^s = \mathbf{b}_0^s \otimes \mathbf{n}_0^s$ and $\mathbf{m}_0^t = \mathbf{b}_0^t \otimes \mathbf{n}_0^t$ are the Schmid tensors associated with slip system $s$ and twin system $t$.

The role of Eq. 11 is to determine whether or not a particular slip system $s$ belonging to specific slip modes becomes active. It introduces $\tau_c^s$, a value for slip resistance of slip system $s$. This resistance is expected to naturally evolve with strain due to many microstructural factors.
and be affected by strain rate and temperature. To account for this variation in slip resistance, or hardening, we employ a thermally activated dislocation density based hardening law (DD model) developed in (Beyerlein et al., 2011a; Beyerlein et al., 2011b; Knezevic et al., 2015b). In this model, the slip resistance changes with the evolution of stored dislocation density. The evolution laws apply to each slip system \( s \) in each slip mode \( \alpha \) and each mode possesses its own dependencies with strain rate and temperature.

Here the hardening model is briefly reviewed in order to introduce the material parameters (e.g., initial slip resistance, activation barriers, drag stress, etc.).

The resistance to slip \( \tau_c^s \) is given by the following sum:

\[
\tau_c^s = \tau_o^\alpha + \tau_{HP}^s + \tau_{for}^s + \tau_{deb}^\alpha,
\]

where \( \tau_o^\alpha \) is a friction stress, \( \tau_{HP}^s \) a barrier term, \( \tau_{for}^s \) a forest dislocation interaction resistance, and \( \tau_{deb}^\alpha \), a substructure interaction resistance. The first term depends on temperature according to:

\[
\tau_o^\alpha(T) = A^\alpha \exp\left(-\frac{T}{B^\alpha}\right),
\]

where \( A^\alpha \) [MPa], and \( B^\alpha \) [K] are material coefficients and \( T \) is temperature in Kelvins [K]. The inverse relationship between the resistance and temperature is common to many other metals as shown in (Beyerlein and Tomé, 2008; Flynn et al., 1961; Knezevic et al., 2014a; Knezevic et al., 2012; Knezevic et al., 2014b; Knezevic et al., 2013d). The second term, \( \tau_{HP}^s \), follows a Hall-Petch-like law via:

\[
\tau_{HP}^s = \mu^\alpha(T)H_{i}^\alpha \frac{b^\alpha}{d_{mfp}^s}.
\]

In Eq. (14), \( b^\alpha \) is the magnitude of the Burgers vector of the dislocations belonging to slip mode \( \alpha \), \( \mu^\alpha(T) \) is the effective shear modulus (Fisher and Renken, 1964), and \( H_{i}^\alpha \) is the Hall-Petch coefficient. The subscript \( i \) defines whether the grain contains primary extension twins \((i=1)\),
primary contraction twins \((i=2)\), or secondary contraction twins within the primary extension twins \((i=3)\). The Burgers vectors are \(3.21 \times 10^{-10} \text{ m}, \ 3.21 \times 10^{-10} \text{ m}, \ \text{and} \ 6.12 \times 10^{-10} \text{ m}\) for basal, prismatic, and pyramidal slip modes, respectively. In this work for AZ31, we use \(\mu^\alpha(T) = 19.5 - 0.012T\) (Watanabe et al., 2004). The length \(d_{mf}^s\) is the mean free path between adjacent twins within the grain and depends on the orientation relationship between the twin boundary and the slip plane as (Beyerlein and Tomé, 2008; Proust et al., 2007) and it is given by:

\[
d_{mf}^s = \frac{(1 - f^{pts})d_c}{\sin(\theta)}
\]  

(15)

where \(f^{pts}\) is the twin fraction of predominant twin system (PTS) in the grain, the angle \(\theta\) is the angle between the slip plane and the plane of the twinning system and \(d_c\) is the twin spacing given by the ratio of the grain size, \(d_g\), to the number of lamellae, which in this work is assigned a nominal value of five. The nominal value of five is used based on observations of average number of twin lamellae per grain including primary and secondary twins. Note that we allow formation of multiple twin variants per grain while still maintaining the concept of a predominant twin system for the calculation of the mean free path (i.e. Eq. 15). However, the volume fraction of the parent grain is transferred to the multiple twin grains that are being formed.

The contributions to slip resistances of \(\tau_{for}^s(\dot{\varepsilon}, T)\) and \(\tau_{deb}^\alpha(\dot{\varepsilon}, T)\) are related to the forest dislocation density \(\rho_{for}^s(\dot{\varepsilon}, T)\) and substructure dislocation density \(\rho_{deb}^\alpha(\dot{\varepsilon}, T)\) according to (Madec et al., 2002; Mecking and Kocks, 1981):

\[
\rho_{for}^s(\dot{\varepsilon}, T) = b^\alpha \mu^\alpha(T) \sqrt{\chi^{ss'} \rho_{for}^{ss'}(\dot{\varepsilon}, T)},
\]  

(16a)

\[
\tau_{deb}^\alpha(\dot{\varepsilon}, T) = k_{deb} \mu^\alpha(T) b^\alpha \sqrt{\rho_{deb}(\dot{\varepsilon}, T)} \log \left( \frac{1}{b^\alpha \sqrt{\rho_{deb}(\dot{\varepsilon}, T)}} \right).
\]  

(16b)
where $\chi^{ss'}$ is a dislocation interaction matrix and $k_{deb} = 0.086$ (Madec et al., 2002). Without loss of generality and to minimize use of parameters with little experimental support, we set the diagonal terms ($s=s'$) to a typical value of 0.81 and the off-diagonal terms to zero (Mecking and Kocks, 1981).

The forest density, $\rho_{for}^s(\dot{\varepsilon}, T)$, evolves according to a balance between the rate of generation/storage and removal/dynamic recovery (Essmann and Mughrabi, 1979; Mecking and Kocks, 1981):

$$\frac{\partial \rho_{for}^s}{\partial \gamma^s} = \frac{\partial \rho_{gen,for}^s}{\partial \gamma^s} - \frac{\partial \rho_{rem,for}^s}{\partial \gamma^s} = k_1^{\alpha} \sqrt{\rho_{for}^s} - k_2^{\alpha}(\dot{\varepsilon}, T)\rho_{for}^s. \quad (17)$$

In Eq. (17), $k_1^{\alpha}$ is a coefficient for dislocation storage by statistical trapping of moving dislocations and $k_2^{\alpha}$ is a coefficient for dynamic recovery by thermally activated mechanisms (e.g., cross-slip and climb). The latter coefficient is given by (Beyerlein and Tomé, 2008),

$$\frac{k_1^{\alpha}}{k_2^{\alpha}} = \left( \chi^{ss'} \right)^{-1} \left( \frac{\tau_{sat}^{\alpha}}{b^\alpha \mu^\alpha} \right)^2, \quad (18a)$$

where

$$\tau_{sat}^{\alpha} = \frac{D^\alpha (b^\alpha)^3 g^\alpha \mu^\alpha}{D^\alpha (b^\alpha)^3 - kT \ln \left( \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \right)}. \quad (18b)$$

In Eq. (18), $k$, $\dot{\varepsilon}_0$, $g^\alpha$, and $D^\alpha$ are the Boltzmann constant, a reference strain rate taken here to be $10^7$ s$^{-1}$, an effective activation enthalpy, and a drag stress, respectively. Note that we have defined the coefficient, $k_2^{\alpha}$, flexible to include the anisotropic interactions through $\chi^{ss'}$. However, accurate characterization of this parameter requires more sophisticated explicit dislocation
models and is left for future work. Debris density increment is coupled to the rate of recovery of all active dislocations through:

\[
d\rho_{\text{deb}} = \sum_i q^\alpha(T)b^\alpha \sqrt{\rho_{\text{deb}}} \frac{\partial \rho_{\text{rem,for}}^{i'}}{\partial \gamma^{i'}} |d\gamma^{i'}|.
\]  

(19)

In Eq. (19), \(q^\alpha(T)\) is a rate parameter defining the fraction of recovered dislocations stored as debris.

2.3.3 Deformation twinning

Deformation twinning is allowed in each of constituent grains at each integration point. To calculate the rate of change of the twin volume fraction per twin system, \(\dot{f}^t\), in Eq. (4b) a pseudo-slip model (Kalidindi, 1998; Van Houtte, 1978) is used. The pseudo-slip model only considers the shear accommodated by twinning, but not for the reorientation or the formation of a twin domain. According to this model, \(\dot{f}^t\), is related to the shear rate on the twin system, according to:

\[
\dot{f}^t = \frac{\dot{\gamma}^t}{S^t},
\]

(20)

or in a given increment by

\[
\Delta f^t = \frac{\Delta \gamma^t}{S^t}.
\]

(21)

When \(\sum_1^n \Delta f^t = 1\), that is, when, in \(n\) strain increments, the volume fraction of a particular twin system, \(t\), reaches unity the system accommodated its maximum shear strain, i.e., \(S^t = \sum_1^n \Delta \gamma^t\).

Similar to slip, the shear strain rate, \(\dot{\gamma}^t\), for each twinning system \(t\) is calculated using the power law relationship between the resolved shear stress \(\tau^t = \mathbf{T}^e \cdot \mathbf{m}_0^t\) on the twinning system to its characteristic resistance \(\tau_c^t\) (Asaro and Needleman, 1985; Hutchinson, 1976; Kalidindi, 1998):
\[
\dot{\gamma} = \begin{cases} 
\dot{\gamma}_0 \left( \frac{\tau}{\tau_c} \right)^m \text{sign}(\tau) & \text{if } \tau > 0 \\
0 & \text{if } \tau < 0 
\end{cases} \tag{22}
\]

As before, \( \dot{\gamma}_0 \) is a reference slip rate (equal to 0.001 s\(^{-1}\)) and \( m \) represents the strain rate sensitivity factor (equal to 0.01).

The flow rule in Eq. (22) introduces a characteristic resistance \( \tau_c \), which is the activation stress for twinning. The resistance \( \tau_c \) is the result of three contributions:

\[
\tau_c = \tau_{o}^\beta + \tau_{0,HP}^\beta + \tau_{slip}^t.
\tag{23}
\]

where the first is a temperature-independent friction term \( \tau_{o}^\beta \),

\[
\tau_{o}^\beta = \tau_{prop}^\beta + (\tau_{crit}^\beta - \tau_{prop}^\beta) \exp \left( -\sum \frac{\rho_{for}^s}{\rho_{sat}^s} \right),
\tag{24a}
\]

with \( \tau_{crit}^\beta \) and \( \tau_{prop}^\beta \) defined as the nucleation and propagation stresses, whose contribution to twin activation is leveraged by the probability term (Beyerlein and Tomé, 2008). The dislocation densities of all slip systems enter into the probability equation \( \sum \frac{\rho_{for}^s}{\rho_{sat}^s} \) in which \( \rho_{sat}^s = \left( \frac{k_1}{k_2} \right)^2 \).

The second contribution is a Hall-Petch-like term \( \tau_{0,HP}^\beta \).

\[
\tau_{0,HP}^\beta = \frac{H_0^\beta}{\sqrt{d_g}},
\tag{24b}
\]

and the last one is a latent hardening term that couples slip and twin systems:

\[
\tau_{slip}^t = \mu^\beta (T) \sum_s C^{\beta\alpha} b^\beta b^\alpha \rho_{for}^s.
\tag{24c}
\]

In Eq. (24), \( \mu^\beta \) is the elastic shear modulus on the system, \( b^\beta \) is the Burgers vector of a given twin system, and \( C^{\beta\alpha} \) is the latent hardening matrix. The six twin variants, \( t \), belonging to the same twin mode, \( \beta \), have their own activation stress and relationship to the dislocations stored within the crystal. The Burgers vectors are \( 1.38 \times 10^{-10} \) m and \( 9.24 \times 10^{-11} \) m for extension and contraction twin modes, respectively.
We use a composite grain (CG) scheme for the lattice reorientation associated with twinning (Proust et al., 2007). In the original CG approach, only one twin phase is allowed per grain, which is usually the predominant twin system (PTS), the twin system with the highest shear-rate among all twin systems. The pseudo-slip model in Eq. (22) was then used to determine when the PTS reached a threshold twin volume fraction. Expansion of the PTS is then modeled by transferring volume fraction from the parent grain to the twin. In the present CG approach, multiple twin variants per grain are allowed. When the twin volume fraction \( f^t \) of a particular twin variant, \( t \), reaches a critical value (which is 1% in these calculations), a twin phase is introduced. As there are six variants for every twin mode and two twin modes are taken into account in the present material model, 12 distinct twin grains per parent grain are permitted, although in actuality, it would be exceedingly rare or impossible that all 12 variants would form in the same grain. Every newly formed twin grain takes on the crystallography of the corresponding twin variant \( t \). As before, the volume of each twin grain is removed from that of the parent. As each twin grain increases in volume, the matrix volume reduces by the same amount. The total sum of volume fractions of the parent and its corresponding twin grains is always one. As an assumption, all twin grains inherit from its parent grain the resistance values for the slip and twinning systems along with the values of the forest and substructure dislocation densities.

3. Model setups and characterization

In this section, the T-CPFE model is used to simulate 20 true stress-true strain curves and concomitant microstructure evolution along with the underlying predictions of crystallographic characteristics in tension, compression, and free-end torsion of AZ31 samples. The model is also
used to simulate geometrical changes during compression of AZ31 samples cut in two perpendicular directions.

For the AZ31 magnesium alloy, the slip modes that have been identified over the years are basal a, prismatic a, pyramidal a, and 2\textsuperscript{nd} order pyramidal c+a modes. Basal a slip is known as the easy slip mode (Roberts, 1960). Prismatic a is harder to activate than basal slip while pyramidal a slip requires even higher driving forces or elevated temperatures (Kelly and Hosford, 1968; Lou et al., 2007; Obara et al., 1973). To accommodate c-axis strains, 2\textsuperscript{nd} order pyramidal c+a slip systems and deformation twinning are the common mechanisms (Agnew and Duygulu, 2004; Agnew et al., 2003; Keshavarz and Barnett, 2006; Muránsky et al., 2008; Obara et al., 1973; Stohr and Poirier, 1972; Yoshinaga et al., 1973). In particular, {\{1012\}1\overline{1}1\overline{1}} extension twins and {\{10\overline{1}1\}\{10\overline{1}\overline{2}\}} contraction twins are most often observed in Mg alloys (Yoo, 1981). These twins produce shear strains of 0.1289 and 0.1377, respectively. The lattice reorientation due to extension twins is a rotation of 86.3° about the {\langle1\overline{1}20\rangle} direction and for contraction twins it is a rotation of 56.2° about the {\langle1\overline{1}20\rangle} direction (Yoo and Lee, 1991).

Figure 2 illustrates the FE meshes used here for the AZ31 deformation simulations. The z-axis of the FE models represents the extrusion direction (ED) of the material. The FE mesh shown in Fig. 2a is a cubic cell consisted of 64 C3D8 (continuum three-dimensional eight-nodal) elements used for identification of hardening parameters and predictions of stress-strain response, texture, and twin volume fraction. Deformation boundary conditions were prescribed by specifying displacements along the loading direction while securing the stress-free boundary conditions on the lateral faces (Jahedi et al., 2015). In addition, simple shear displacement boundary conditions in the ED plane were prescribed for the simulation of free end torsion. The displacement was applied in the y-direction while preventing any expansions in x- and z-
directions. Figure 2b shows $1/8$th of a cylinder consisting of 660 C3D8 elements used to simulate cylinder compressions. Symmetry boundary conditions were applied to the three faces along which the cuts were made. The same deformation of the model was prescribed i.e., displacement along the loading direction while ensuring the stress-free boundary conditions on the lateral faces.

The starting material consisted of nearly equiaxed grains with an average diameter of 13 µm. The material model is initialized with the measured initial texture given in (Kabirian et al., 2015). The texture is based on the neutron diffraction measurements and is shown in Fig. 2c. The initial texture was typical of an extruded Mg alloy in which the (1010) poles were highly aligned along the ED-direction and the basal poles were approximately uniformly lying in the ED-plane. The texture was represented using 3,168 crystal orientations, which were imported into the model via random assignment to the Taylor polycrystals. We use $N = 6$ grains for the Taylor cluster at each integration point to start the model identification (Fig. 2a). The imposed strain rate and temperature in each test is consistent with the experiments. The same starting texture was used to initialize the cylinder compression simulations (Fig. 2b). However, 80 crystal orientations were used at each integration point totaling to 422,400. Every orientation is allowed to develop multiple twin variants and, therefore, the number of orientations at each integration point increases with strain very quickly.
Figure 2 Finite element models for simple compression simulations: (a) cubic cell consisted of 64 C3D8 (continuum three-dimensional eight-nodal) elements used for identification of hardening parameters, (b) 1/8 of the cylindrical billet consisted of 660 C3D8 used for anisotropic material flow predictions, and (c) pole figures of the initial texture. Every integration point initially embodies in (a) 6 crystal orientations totaling to 3,168 and in (b) 80 crystal orientations totaling to 422,400. Every orientation is allowed to develop multiple twin variants and, therefore, the number of orientations at each integration point increases with strain very quickly.

The multi-level model developed here is applied to identify the underlying slip and twinning mechanisms responsible for the plastic anisotropic behavior of AZ31 Mg and physical material parameters governing slip. The experimental data are reported in (Kabirian et al., 2015). There the authors provide a comprehensive set of responses under distinct loading states and a wide range of temperatures (77K to 423K) and strain rates (10^{-4} s^{-1} to 3000 s^{-1}). Twenty stress-strain responses reported there are considered in this work. These consist of compression tests in two directions: 0° and 90° to the ED, each at three temperatures and three strain rates; and one torsion test and one ED-tension test at 10^{-4} s^{-1} and room temperature (298K). Half the curves were used for calibration while the other half can be regarded as predictions. The goal is to capture these 20 deformation responses with a single set of material parameters.

4. Results

In this section, we present the simulation results for flow stress, deformation texture, twinning, and sample geometry changes with strain and compare them with experiments.
4.1 Stress-strain response

We first compare the constitutive responses calculated with the measured ones. Following the work reported in (Kabirian et al., 2015), we denote the 0° and 90° compression tests as ED and PED, respectively.

The stress-strain responses in ED-tension and ED-torsion were used to obtain approximate values of material parameters initially for specific slip modes, because the material in these cases deform predominantly by slip. However, due to the initial texture the deformation also exhibit a small amount of twinning. These values were then slightly corrected during calibration of the other compression curves along with estimating the twinning parameters. At least four stress-strain curves can be regarded as model predictions.

Figure 3a compares the measured and calculated responses for the ED-compression tests. As shown, the model captures well the effects of temperature and strain rate on the stress-strain response with respect to flow stress and hardening. All ED-compression curves exhibit a sigmoidal shape, a well-known signature of profuse twinning activity. An interesting feature is the relatively small effect of changing the temperature from 77K to 298K in the deformation response for the two lower strain rates $10^{-4}$ s$^{-1}$ and 1 s$^{-1}$. The high-rate response, in contrast, shows a noticeable dependency on temperature. The sigmoidal shape at 3000 s$^{-1}$ is not as pronounced as it is at lower strain rates resulting in the steep hardening due to twinning starting earlier. The model successfully captures well these shifts in hardening as a function of strain rate and temperature.

Figure 3b compares the measured and calculated responses for the PED-compression tests. In the model, the only change made was in the prescribed loading direction, which is now perpendicular to the extrusion direction rather than along it (i.e., y-axis). The same starting
texture and material constitutive laws were used. Due to strong initial texture, we can expect that the behavior in this loading direction will be different than the ED-compression tests under the same conditions. One clear difference is that the hardening rates are lower and the sensitivity to temperature is stronger, the characteristics of more thermally activated glide than deformation twinning accommodated deformation. Although some of these responses exhibit the common twin signature of inflections in hardening and a high hardening rate, these signs are not as pronounced as in the ED-compression tests. In fact, for the deformation responses at both the quasi-static rate ($10^{-4}$ s$^{-1}$) and at the highest rate (3000 s$^{-1}$) and the highest temperature, 423K, it is not readily apparent whether or not twinning was active. The curves appear to be dominated by slip, in which hardening rates decrease with an increase in strain. Of particular interest here is the fact that the model with the same material parameters agrees with both the ED-compression and PED-compression constitutive responses. The underlying mechanisms associated with these responses are part of the output from this model and these will be discussed shortly.

Figure 3c and d compares the measured and calculated responses for two additional quasi-static, room temperature tests. One is ED-tension. In the model, the boundary conditions were the same as the ED-compression tests except the direction of loading along the ED is reversed from tension. The stress-strain curve in ED-tension exhibits dramatic differences than in ED-compression. This is a well-known tension-compression asymmetry of highly texture Mg alloys (Agnew et al., 2006; Khan et al., 2011; Knezevic et al., 2010) and has been appropriately attributed to activation of extension twinning in one sense (ED-compression) and suppression of twinning and the predominance of slip in the other sense (ED-tension in this case). Therefore the tensile curve exhibits the typical decreasing strain hardening rate. Another is free-end-torsion in extrusion direction (ED) plane. The strain hardening response during the free-end torsion is
similar to that in tension with the shear yield stress significantly smaller than in tension. The model captures this test with good accuracy to high strain levels. It is expected that the model can be easily extended to simulate the response at even broader ranges of strain rates and temperatures.

**Figure 3** True stress-true strain responses of extruded and annealed samples of AZ31 Mg alloy as a function of temperature and strain rate. The loading directions are indicated in the figure: (a) compression in extrusion direction (ED), (b) compression in perpendicular to extrusion direction (PED), (c) tension in extrusion direction (ED), and (d) free-end-torsion in extrusion direction (ED) plane. Measurements are solid lines and predictions are dashed lines.

(a) ED - compression

(b) PED - compression
All deformation responses, ED, PED, ED-tension and torsion, were calculated using the same set of material parameters, which is given in Table I and II. This set is anticipated to be reliable since matching such a large number of diverse responses severely constrains the model. As a means of comparing to prior values from other modeling studies on AZ31, we consider the initial characteristic strengths $\tau_0^{\alpha}$, without the effects of dislocation-dislocation and dislocation-boundary interactions, which is common to all these models. Referring to Table I, we find that the ratios of the initial activation stresses for basal $\langle a \rangle$ to prismatic $\langle a \rangle$ to pyramidal $\langle c + a \rangle$ to the $\{10\overline{1}2\}\{10\overline{1}1\}$ twin mode were 1:4.1:14:1.2 at room temperature. In prior studies using Voce hardening for modeling of AZ31 at room temperature, these ratios were found to be 1:5:6:2 in (Cizek and Barnett, 2008), 1:15:22.5:1.25 in (Kabirian et al., 2015), 1:3.2:5:1.5 in (Jain and Agnew, 2007), 1:5.5:6:3 in (Agnew et al., 2003). A more detailed summary of the CRSS values from literature for Mg alloys either measured or inferred by modeling is given in (Hutchinson and Barnett, 2010; Lou et al., 2007). In a recent study (Wang et al.) the authors used nearly the same dislocation density evolution law as here but in an elastic visco-plastic SC (E-VPSC) framework and they found 1:4:13:1.4. Generally, these estimates are qualitatively, but not quantitatively similar. The values reported in the present paper were calibrated and validated to the most comprehensive data set reported thus far.

\[ \dot{\varepsilon} = 10^{-4} \text{ s}^{-1} \]

\[ \dot{\varepsilon} = 10^{-4} \text{ s}^{-1} \]
Table I Model parameters used for the evolution of slip system resistances.

<table>
<thead>
<tr>
<th>α – slip mode</th>
<th>Basal slip</th>
<th>Prismatic slip</th>
<th>Pyramidal slip</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tau_0^\alpha ) [MPa]</td>
<td>( 17 \exp(-T/786) )</td>
<td>( 108 \exp(-T/359) )</td>
<td>( 290 \exp(-T/489) )</td>
</tr>
<tr>
<td>( k_1^\alpha ) [m(^{-1})]</td>
<td>( 6 \times 10^6 )</td>
<td>( 9.8 \times 10^7 )</td>
<td>( 1.5 \times 10^8 )</td>
</tr>
<tr>
<td>( g^\alpha )</td>
<td>( 6.4 \times 10^{-4} )</td>
<td>( 1.2 \times 10^{-4} )</td>
<td>( 6.2 \times 10^{-3} )</td>
</tr>
<tr>
<td>( D^\alpha ) [MPa]</td>
<td>100</td>
<td>150</td>
<td>225</td>
</tr>
<tr>
<td>( q^\alpha )</td>
<td>( 42 \ln(1 + T/14) )</td>
<td>( 130 \ln(1 + T/10) )</td>
<td>( 140 \ln(1 + T/10) )</td>
</tr>
<tr>
<td>( H_1^\alpha ) [MPa]</td>
<td>10</td>
<td>195</td>
<td>510</td>
</tr>
<tr>
<td>( H_2^\alpha ) [MPa]</td>
<td>200</td>
<td>350</td>
<td>1000</td>
</tr>
<tr>
<td>( H_3^\alpha ) [MPa]</td>
<td>450</td>
<td>1850</td>
<td>3000</td>
</tr>
</tbody>
</table>

Table II Model parameters used for the evolution of twin system resistances.

<table>
<thead>
<tr>
<th>β – twin mode</th>
<th>Extension twins</th>
<th>Contraction twins</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tau^\beta_{\text{crit}} ) [MPa]</td>
<td>13</td>
<td>135</td>
</tr>
<tr>
<td>( \tau^\beta_{\text{prop}} ) [MPa]</td>
<td>5</td>
<td>130</td>
</tr>
<tr>
<td>( \tau^\beta_0 ) [MPa]</td>
<td>12.8</td>
<td>136</td>
</tr>
<tr>
<td>( H_0^\beta ) [MPa]</td>
<td>30</td>
<td>85</td>
</tr>
<tr>
<td>( C^{\alpha \beta}, \alpha=1 )</td>
<td>850</td>
<td>200</td>
</tr>
<tr>
<td>( C^{\alpha \beta}, \alpha=2 )</td>
<td>400</td>
<td>300</td>
</tr>
<tr>
<td>( C^{\alpha \beta}, \alpha=3 )</td>
<td>300</td>
<td>400</td>
</tr>
</tbody>
</table>

The predicted variation in \( \tau_0^\alpha \) with temperature is given in Fig. 4 with numerical values given in Table III. It can be seen that different modes exhibit different dependence on temperature. Also, the relative ratios decrease with temperature. We see that basal slip is the least sensitive to
temperature, which is consistent with measurements performed on single crystals reported in (Akhtar and Teghtsoonian, 1969a). Prismatic slip shows more temperature dependence, which is also consistent with measurements (Akhtar and Teghtsoonian, 1969b). Finally, pyramidal \( (c + a) \) slip is the most sensitive. It can, therefore, be expected that plastic deformation behavior that is predominantly carried by basal slip would be less sensitive temperature than that which is predominantly supported by pyramidal \( (c + a) \) slip. The same large sensitive of \( (c + a) \) slip to temperature is seen in other HCP metals, such as Zr (Beyerlein and Tomé, 2008; Zecevic et al., 2015a).

Grain size strengthening effects are typically accounted by the Hall-Petch relationship. The mechanism is understood in terms of dislocation pile-ups in the vicinity of the grain boundary. It was found that AZ31 exhibits a significant variation in the Hall-Petch slope, which is explained by texture effects (Barnett et al., 2004; Yuan et al., 2011). This suggests that the Hall-Petch terms should be associated with a particular dislocation type as was done in the present modeling effort. The values established for twin free grains, particularly those for basal slip, which is the easiest to activate, lie within the range of experimentally observed scatter. The values for grains containing twins are fit for the first time here to reproduce the macroscopic stress-strain curves. In particular, the Hall-Petch-like term associated with contraction twins as secondary twins is higher than that for extension twinning. This trend agrees with the recent finding that the thin contraction twins cause strain hardening since they decrease the mean-free-path of the pyramidal \( (c + a) \) dislocations (Knezevic et al., 2010).
Figure 4 Initial values of slip system resistances as a function of temperature.

Table III Initial values of slip system resistances as a function of temperature.

<table>
<thead>
<tr>
<th>$\tau_0^\alpha$ [MPa]</th>
<th>Basal slip</th>
<th>Prismatic slip</th>
<th>Pyramidal slip</th>
</tr>
</thead>
<tbody>
<tr>
<td>77 K</td>
<td>16</td>
<td>88.4</td>
<td>255.9</td>
</tr>
<tr>
<td>298 K</td>
<td>11</td>
<td>45.5</td>
<td>154.7</td>
</tr>
<tr>
<td>423 K</td>
<td>10.5</td>
<td>34.1</td>
<td>129.2</td>
</tr>
</tbody>
</table>

4.2 Evolution of twinning and texture

In the foregoing section, the stress-strain curves were used to characterize the hardening parameters and activation stresses needed for twinning. In this section, we will use other experimental microstructure data to validate the model. Specifically, we compare the results with measurements of twin volume fraction, deformation textures, and lateral strain measurements made on deformed samples.

We first consider the extension twin volume fraction measured in the ED test at room temperature and $10^{-4}$ s$^{-1}$. Figure 5 shows the measurements taken from (Kabirian et al., 2015) alongside the calculated variation in twin volume fraction with strain. This particular test involved a substantial amount of twinning, from 0 to 50% volume fraction developing over the
first 10% of straining. As seen, the model provides good agreement in the amount of twinning and its rate of growth.

![Graph showing twin volume fraction vs. true strain](image)

**Figure 5** Evolution of the twin volume fraction during compression in extrusion direction (ED) at 298 K and under a strain rate of $10^{-4}$ s$^{-1}$ predicted by the model (line) and measured by neutron diffraction (symbols).

As another validation metric, we compare the model predictions with texture measurements made on deformed samples. In (Kabirian et al., 2015), deformation textures were measured for a few of the ED-compression and PED-compression tests after straining to several strain levels. Figure 6 presents side-by-side the textures from the model and measurements.

<table>
<thead>
<tr>
<th>Measured</th>
<th>Simulated</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a) ED - compression</td>
<td></td>
</tr>
<tr>
<td>$\varepsilon = 0.1$, $T = 298K$, $\dot{\varepsilon} = 10^{-4}$ s$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$\varepsilon = 0.065$, $T = 298K$, $\dot{\varepsilon} = 3000$ s$^{-1}$</td>
<td></td>
</tr>
</tbody>
</table>
(b) PED - compression

$\varepsilon = 0.055, T = 423K, \dot{\varepsilon} = 10^{-4} \text{ s}^{-1}$

$\varepsilon = 0.055, T = 423K, \dot{\varepsilon} = 1 \text{ s}^{-1}$

$\varepsilon = 0.055, T = 423K, \dot{\varepsilon} = 3000 \text{ s}^{-1}$

$\varepsilon = 0.025, T = 298K, \dot{\varepsilon} = 10^{-4} \text{ s}^{-1}$

$\varepsilon = 0.055, T = 298K, \dot{\varepsilon} = 3000 \text{ s}^{-1}$

$\varepsilon = 0.055, T = 423K, \dot{\varepsilon} = 10^{-4} \text{ s}^{-1}$
Figure 6 Pole figures showing comparison of the measured and predicted texture evolution of AZ31 deformed in compression along (a) extrusion direction (ED) and perpendicular to extrusion direction (PED) to the strain levels and under temperatures and strain rates indicated in the figure.

In ED-compression, despite the differing test conditions of temperature and strain rate, the most prominent change is the re-alignment of the basal poles to along the ED. This change diverges significantly with the initial texture (Fig. 2c) and is a strong signature of \{\overline{1}012\}\{10\overline{1}1\} twinning. Compared to the room temperature tests, in the deformation textures from the high temperature tests, the basal pole maximum along the ED is slightly less intense. This difference is explained by slightly less tensile twinning activity and more slip activity in the high temperature loading conditions. Experimental measurements reported in (Jain and Agnew, 2007) show that there is very little to no variation in twin activity up to the temperature of 423 K. With further increase in temperature, the twinning activity substantially decreases (Jain and Agnew, 2007).

Like the textures that develop in ED-compression, the PED-compression textures appear to also be a result of extension twinning and slip. The basal poles have re-aligned along the PED,
which is the direction of loading perpendicular to the ED-compression test, and again is a clear signature of \{\overline{1}012\}\langle10\overline{1}1\rangle twinning. This texture change persists in all temperatures and strain rates.

4.3 Evolution of geometry during compression

As a third form of validation, we compare the lateral deformation of the deformed cylinder predicted by the model with the measurement. The measurements were carried out for ED-compression and PED-compression at room temperature and a strain rate of $10^{-4}$ s$^{-1}$. For different levels of applied compression strain, the lateral strains in the two in-plane orthogonal directions were measured, $\varepsilon_{11}$ and $\varepsilon_{22}$. Figure 7a compares the calculated evolution of $\varepsilon_{11}$ and $\varepsilon_{22}$ with axial strain with the experimental measurements for these two tests. The model not only captures the rate of $\varepsilon_{11}$ and $\varepsilon_{22}$ in both tests, but the more profound ovalization in the PED-compression tests than in the ED-compression tests. Specifically in the PED-compression tests, $\varepsilon_{11}$ is much greater than $\varepsilon_{22}$.

The geometrical changes of the samples compressed to a strain of 0.1 are shown in Fig. 7b and c. Here, the symbols overlaid onto the photographs of the deformed cross sections denote the external nodal coordinates of the deformed FE model predictions. We see that the ED-compression sample preserved a near uniform cross-section but the PED-compression sample developed an oval cross-section. It is worth mentioning that model agreement in the geometric changes to the cylindrical sample is a strong validation of the T-CPFE UMAT implementation and its ability to predict texture-induced, anisotropic material flow of a material that slips and twins.
Figure 7 (a) Comparison of measured (symbols) and simulated (lines) evolution of lateral strains during compression along extrusion direction (ED) and perpendicular to extrusion direction (PED). Top view of the compression samples after 0.1 strain level compressed in (b) ED and (c) PED. The external nodal coordinates of the deformed FE models are superimposed on the experimentally deformed samples of AZ31.

5. Discussion

In addition to the evolution of flow stress, microstructural, and texture with strain, the T-CPF model can provide useful insight on the active slip and twin modes predominating each deformation response. To extract this information from the calculation, we choose to analyze the change in the relative slip and twin activities with applied strain. Here, the relative activity of a slip or twin mode in a given grain of the polycrystal is defined as the fraction of the grain strain accommodated by the active slip (twin) systems belonging to mode. For a slip mode $\alpha$, the relative activity is given by:

$$\text{Relative activity}^{\alpha} = \frac{\sum_\alpha \dot{\gamma}^s}{\sum_s \dot{\gamma}^s + \sum_t \dot{\gamma}^t}.$$  

(25)
The denominator in Eqn (25) is the sum over all active slip and twin systems in that grain. For the entire sample, the relative activity is then averaged over all grains in the Taylor polycrystal at an FE integration point, which is then averaged over all integration points in the FE model.

Figure 8 shows the slip and twin activities in the ED-compression, PED-compression, ED-tension, and ED-torsion tests. Each relative activity plot per sample consists of two plots: one for the mode activity within the parent material and one for the mode activity within the twinned material. The results show that in all cases, the deformation is accommodated by a combination of slip and twinning. The clear differences in flow stress-strain evolution among these tests result from differing relative amounts of slip and twinning activity. For the ED-compression and PED-compression responses, only the 298 K at $10^{-4}$ s$^{-1}$ cases are displayed because the activities at the 77 K and 423 K and at higher strain rates were qualitatively similar to those at 298 K and $10^{-4}$ s$^{-1}$.
Figure 8 Predicted relative activities of each deformation mode contributing to plasticity in both the parent grains (on the left) and the twins (on the right) for the samples deformed as indicated in the figure at $T = 298$ K and $\dot{\varepsilon} = 10^{-4}$ s$^{-1}$. Plotted is the parent and twinned material volume fraction.

The slip activities for the ED-compression tests are given in Fig. 8a. As shown, the most active system initially is basal slip. Prismatic slip becomes more active than basal slip with further straining. The active slip systems and their relative contributions are not surprising given the load orientation with respect to the sample texture and their relative resistances. The contribution of $\{\overline{1}0\overline{1}2\}\{10\overline{1}1\}$ twinning explains the re-alignment of the basal poles along the ED seen in the texture measurements. Interestingly, their contributions do not change substantially with temperature and strain rate. Activity of twinning has been observed not to substantially change up to 423 K and with strain rate (Jain and Agnew, 2007; Watanabe and
Ishikawa, 2009). This result clarifies why the texture was observed to develop in a similar way among all the ED-compression tests.

In Fig. 8b, we show the relative activities of slip and twinning in the PED-compression tests. We find that this deformation response is predominantly accommodated by basal slip. Compared to the ED-compression response, the PED-compression response has less contributions of \{\bar{1}012\}(10\bar{1}1) twinning and prismatic slip. The contribution of \{\bar{1}012\}(10\bar{1}1) explains the realignment of the basal poles along the PED. The basal slip dominance is maintained despite large changes in strain rate and temperature. The model predicts only small decreases in basal slip activity and increases in pyramidal \(c + a\) activity as strain rate increases from \(10^{-4}\) s\(^{-1}\) to 3000 s\(^{-1}\).

As seen in these results, in all the ED-compression and PED-compression conditions, the simulations indicate the activation of extension twinning. We also find that within these reoriented \{\bar{1}012\}(10\bar{1}1) twin domains, pyramidal \(c + a\) slip becomes the dominant slip system. In some instances, pyramidal \(c + a\) slip is also accompanied by contraction twinning. It has been found that the thin contraction twins are effective in strain hardening of the alloy by decreasing the mean-free-path of pyramidal \(c + a\) dislocations (Knezevic et al., 2010). Our simulations support this finding since the Hall-Petch term associated with contraction twins as secondary twins is much higher than that for the extension twinning. Internal \{10\bar{1}1\}(10\bar{1}2) contraction twinning within the primary \{\bar{1}012\}(10\bar{1}1) extension twin domains is commonly seen to be a precursor for tertiary twinning; that is, when extension twinning occurs within the secondary contraction twin domain (Lentz et al., 2014; Mu et al., 2012). However, the tertiary twins often occur in very tiny volume fractions that could not be expected to be detectable in a bulk texture measurement.
The tension-compression asymmetry seen in the flow response in AZ31 is well known to arise from noticeable differences in the relative activities of slip and twinning and their contribution to hardening. From the model predictions for ED-tension in Fig. 8c, we see that the slip systems active in ED-tension are different than in ED-compression. First, in ED-tension, the orientation of the \(c\)-axis relative to the loading direction is such that the \(c\)-axes of most grains are compressed. Accordingly extension twinning is largely suppressed. It would be expected that in its place, pyramidal \(\langle c+a\rangle\) or contraction twinning could operate. The model finds that contraction of the \(c\)-axis in ED-tension is mostly accommodated by pyramidal \(\langle c+a\rangle\) and very little contraction twinning. Because pyramidal \(\langle c+a\rangle\) slip is a harder slip mode to activate compared to \{012\}(10\bar{1}1) twinning, the flow stress is noticeably higher in ED-tension than in ED-compression. ED-compression and ED-tension appear to exhibit similar relatively activity of prismatic slip and basal slip. Last, we mention that the model predicts an increase in tensile twinning activity to \(\sim 10\%\) volume fraction near the end of deformation. \{012\}(10\bar{1}1) twinning activity arises as a result of slip-induced grain reorientation. In other words, after some amount of deformation (\(\sim 10\%\) in this case), some crystals have oriented via plastic slip to an orientation that favors \{012\}(10\bar{1}1) twinning. The relative activities during free-end-torsion resemble those in tension with some increase in basal slip activity and decrease in pyramidal slip activity.

Finally, we return to the mechanisms underlying the geometric changes in the cylindrical samples under ED-compression and PED-compression, discussed earlier in Fig. 7. Based on the initial texture, it would be expected that for ED-compression, \(\varepsilon_{11}\) and \(\varepsilon_{22}\) were likely to be accommodated by similar deformation mechanisms resulting in a similar extension twinning activity. For PED-compression, \(\varepsilon_{11}\) is only likely to be accommodated by extensive extension
twinning activity while $\varepsilon_{22}$ is a crystallographically harder direction dominated by prismatic slip.

6. Conclusions

In this work, we developed a multi-level model for polycrystalline metals that deform by slip and deformation twinning, termed T-CPFE. The macro level employs FE homogenization and the meso level uses a Taylor-type model. The meso level model integrates a new twinning model for handling multiple twin variants per grain. The particular methodology for twinning is the total Lagrangian numerical scheme combined with the advanced composite grain twinning model. The grain level model features a dislocation density based hardening law.

For demonstration, the model is applied to AZ31, an Mg alloy. We calibrated and validated the model on a comprehensive data set collected in compression, tension, and torsion for extruded AZ31 alloy over temperature ranging from 77 K to 423 K and strain rates ranging from $10^{-4}$ s$^{-1}$ to 3000 s$^{-1}$ from (Kabirian et al., 2015). Good agreement between the predicted and measured stress-strain responses, twin volume fraction and texture evolution is achieved. The model indicates that differences in flow stress and microstructure evolution result from differing relative amounts of slip and twinning activity. The relative activities of these systems are found not to be strongly sensitive to strain rate and temperature within the studied ranges. The T-CPFE model is also used to simulate the dimensional changes of the cylindrical AZ31 sample during simple compression. The model successfully predicts the deformed shape of the cylinders, which is demonstrated by direct comparison of the predictions and experimental measurements. This is because the T-CPFE model is able to capture anisotropy and tension–compression asymmetry of the material flow resulting from microstructure evolution and crystallographic mechanisms with
great accuracy. As presented here, this modeling framework is sufficiently general that it can be applied to other polycrystalline materials deforming by slip and twinning.

**Acknowledgements**

This research was sponsored by the Army Research Laboratory and was accomplished under Cooperative Agreement Number W911NF-15-2-0084. IJB would like to acknowledge support through a Los Alamos National Laboratory Directed Research and Development (LDRD) project ER20140348. The authors would like to thank Dr. Farhoud Kabirian and Prof. Akhtar S. Khan for supplying the raw data sets from their article.

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Chapter 2

This chapter was published as: A dislocation density based crystal plasticity finite element model: Application to a two-phase polycrystalline HCP/BCC composites, Milan Ardeljan, Irene J. Beyerlein, Marko Knezevic, Journal of the Mechanics and Physics of Solids, 66, 16-31. My role in preparing this chapter was to numerically implement the developed crystal plasticity finite element model for two-phase polycrystalline HCP/BCC composites whose mechanical behavior was governed by the evolution of dislocation densities. Next, I successfully applied the model to HCP/BCC Zr/Nb layered composite. I contributed in the process of writing the paper by generating and preparing all the relevant figures and creating the specific sections that describe the modeling efforts that were made to model rolling of the two-phase layered composite.
A dislocation density based crystal plasticity finite element model: Application to a two-phase polycrystalline HCP/BCC composites

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Abstract

We present a multiscale model for anisotropic, elasto-plastic, rate- and temperature-sensitive deformation of polycrystalline aggregates to large plastic strains. The model accounts for a dislocation-based hardening law for multiple slip modes and links a single-crystal to a polycrystalline response using a crystal plasticity finite element based homogenization. It is capable of predicting local stress and strain fields based on evolving microstructure including the explicit evolution of dislocation density and crystallographic grain reorientation. We apply the model to simulate monotonic mechanical response of a hexagonal close-packed metal, zirconium, and a body-centered cubic metal, niobium, and study the texture evolution and deformation mechanisms in a two-phase Zr/Nb layered composite under severe plastic deformation. The model predicts well the texture in both co-deforming phases to very large plastic strains. In addition, it offers insights into the active slip systems underlying texture evolution, indicating that the observed textures develop by a combination of prismatic, pyramidal, and anomalous basal slip in Zr and primarily \{110\}\{111\} slip and secondly \{112\}(111) slip in Nb.

Keywords: Dislocations; Texture; Interfaces; Crystal plasticity; Finite elements; Accumulative roll bonding
1. Introduction

Two-phase metal multilayered composites are gaining much interest due to enhanced properties, such as strength and radiation resistance, compared to their constituents. Many of these exciting results arose from research on small-scale thin film composites made by bottom-up processing such as deposition techniques (Anderson et al., 2003; Beyerlein et al., 2013a; Beyerlein et al., 2013c; Chu and Barnett, 1995; Embury and Hirth, 1994; Ham and Zhang, 2011; Mara et al., 2008; Misra and Kung, 2001; Was and Foecke, 1996). It has also been demonstrated that top-down metal working techniques can make large-scale (bulk) composites of similar composition and architecture as deposited films for a number of material systems: Cu/Ag (Han et al., 1999; Ohsaki et al., 2007), Cu/Nb (Carpenter et al., 2012a; Lee et al., 2012; Segal et al., 1997; Zheng et al., 2013), Al/Zn (Dehsorkhi et al., 2011), Cu/Ni (Liu et al., 2011), Ag/Fe (Yasuna et al., 2000) and Zr/Nb (Knezevic et al., 2013b; Knezevic et al., 2014b). Some of these have been tested and found to exhibit high hardness, excellent radiation resistance, good shock resistance and outstanding thermal stability (Beyerlein et al., 2013b; Carpenter et al., 2014; Carpenter et al., 2012b; Han et al., 2014; Monclús et al., 2013). However, unlike the deposited multilayers, these bulk composites experience substantial changes in microstructure, such as texture, grain shape, grain boundary properties, bimetal interface and internal grain dislocation storage due to the large-strain processing (Carpenter et al., 2014; Carpenter et al., 2012a; Knezevic et al., 2013b; Saito et al., 1999; Valiev and Langdon, 2006; Xue et al., 2007). Thus, it is important to understand and have the ability to predict the microstructure and texture evolution in composites under large strain deformations.

For this purpose, several plasticity models have been developed and applied to two-phase composites. Some works have applied mean-field polycrystalline schemes, by either treating the
phases separately or as a homogeneous medium with the appropriate volume fractions of each phase (Beyerlein et al., 2011a; Knezevic et al., 2014b). In these codes, however, the effects of co-deformation at the interface on texture evolution were not modeled explicitly. Any possible adjustments in slip activity or lattice reorientation of the two grains on either side of the interface were missed. Spatially resolved polycrystal codes such as crystal plastic finite element models (CPFE) (Kalidindi et al., 1992; Kalidindi et al., 2009; Knezevic et al., 2010; Roters et al., 2010) and Green’s function fast Fourier transform (FFT) models (Eisenlohr et al., 2013; Lebensohn et al., 2012) can potentially overcome many of the above-mentioned shortcomings. These classes of techniques directly model the grain microstructure and the effects of grain-grain interactions on local granular stress and strain fields. Many of the earlier studies applied CPFE to single-phase materials to capture grain neighbor effects (Diard et al., 2005; Kalidindi et al., 2004; Kalidindi et al., 2006; Roters et al., 2010; Zhao et al., 2008). A few recent studies, however, have used CPFE to study the deformation in two-phase systems (Hansen et al., 2013; Jia et al., 2013; Mayeur et al., 2013). Hansen et al. (Hansen et al., 2013) showed that CPFE can successfully predict the evolution of texture in roll-bonded Cu-Nb with polycrystalline layers. CPFE has also been used to study the onset of shear banding in Cu/Nb and Cu/Ag bicrystals (Jia et al., 2013). A recent study of Cu/Nb bicrystals (Mayeur et al., 2013) explored the stability of interface character under rolling deformation. Notably, the interfaces deemed “stable” by this CPFE model coincided with those observed experimentally to prevail in nano-layered Cu/Nb composites. A subsequent CPFE study of two-phase composites with polycrystalline layers revealed that the orientational stability of grains attached to the interface deviated from those within the bulk layers (Mayeur et al., 2014).
We note that most of the foregoing two-phase studies involve combinations of cubic metals: either two immiscible fcc metals or an fcc and bcc metal. Similar modeling studies on hcp materials (Knezevic et al., 2010) or two-phase combinations involving hcp metals are limited (Venkataramani et al., 2008). The plasticity of hcp metals is more complex than that of cubic materials. In HCP metals, there are several slip and twin modes, each corresponding to planes of different atomic density. The main slip modes are basal \( \langle a \rangle \) slip, \( 1/3 \langle 1\bar{1}20 \rangle \{0001\} \), prismatic \( \langle a \rangle \) slip, \( 1/3 \langle \bar{1}\bar{1}20 \rangle \{\bar{1}100\} \), and pyramidal \( \langle c + a \rangle \) slip, of which there are two types: \( 1/3 \langle 1\bar{1}2\bar{3} \rangle \{1\bar{1}22\} \) or \( 1/3 \langle \bar{1}\bar{1}23 \rangle \{10\bar{1}1\} \) (Partridge, 1967; Yoo, 1981; Yoo et al., 2002). The dislocations associated with these different slip modes possess different atomic core structures (Bacon and Vitek, 2002; Hirth and Lothe, 1968), and their mobilities have their own individual dependencies on temperature and strain rate (Beyerlein et al., 2011b). The development of spatially resolved, polycrystalline models, such as CPFE, for two-phase hcp-based systems presents a new challenge in modeling of multilayered composites to large plastic strains.

1.1 Objectives

The goal of this work is to develop a 3D multi-scale code for bi-phase polycrystalline metals, where the crystal structures may include combinations of fcc, bcc, and hcp. Unlike prior 3D versions, this code employs at the meso-scale, a crystal plasticity finite element homogenization, and at the sub-grain scale, a constitutive law governed by the evolution of dislocations on individual slip systems. As a full field model satisfying both stress equilibrium and strain compatibility, CPFE is expected to provide better predictions of local and overall behavior and microstructure evolution of materials containing co-deformation of multiple phases. In this framework, polycrystalline phases are discretized into finite elements and a single crystal hardening law operates at each FE integration point. To describe the resistance to slip for
individual slip systems in the individual crystals as a function of strain, temperature, and strain rate, we employ a dislocation density (DD) based hardening law developed in (Beyerlein and Tomé, 2008). The model includes two populations of DD: forest dislocations mainly responsible for hardening up to and including stage III and substructure dislocations mainly responsible for hardening stage IV. To model extremely large strains, we present a technique to pass key state variables, the crystal orientation and dislocation density, from the deformed (old) to the undeformed (new) mesh.

In prior work, the DD hardening model has been successfully applied to several metals, differing in crystal structure, such as Haynes 25 (Knezevic et al., 2014a), Nb (Knezevic et al., 2014b), Mg (Beyerlein et al., 2011c), Zr (Beyerlein and Tomé, 2008; Capolungo et al., 2009b; Knezevic et al., 2013b), Be (Knezevic et al., 2013a), and even uranium (Knezevic et al., 2012; Knezevic et al., 2013d; Knezevic et al., 2013e). However in these prior studies, the DD hardening model was incorporated into a visco-plastic self-consistent scheme (VPSC) in order to relate single crystal deformation to the polycrystalline aggregate (e.g. Beyerlein et al., 2011b; Knezevic et al., 2013c; Lebensohn et al., 2007). The VPSC model belongs to a class of more advanced mean-field polycrystal schemes compared to Taylor-type schemes (Al-Harbi et al., 2010; Fast et al., 2008; Knezevic et al., 2009; Knezevic and Kalidindi, 2007; Knezevic et al., 2008; Knezevic and Savage, 2014; Shaffer et al., 2010; Taylor, 1938; Wu et al., 2007) but still cannot capture the effects that grain-to-grain interactions may have on mechanical response and texture evolution. It also cannot model the development of heterogeneities in stress and strain within grains and at grain boundaries and the bimetal interface. To overcome the limitations of mean-field models, the DD model is implemented into a 3D CPFE framework. The combined 3D DD-CPFE model enables predictions of spatially resolved stress and strain fields based on
dislocation density and grain reorientation. Earlier studies found that while alterations in these fields near grain boundaries for some grain orientations can be calculated as a function of certain crystallographic relationships (i.e., the Schmid factor across the interfaces) and applied deformation conditions (temperature and strain rate) using simpler Voce type (Voce, 1948) hardening laws and CPFE kinematics (Acharya and Beaudoin, 2000; Beaudoin et al., 1995; Beaudoin et al., 1996; Raabe et al., 2001; Raabe et al., 2002), for many orientations the kinematic treatment of grain boundaries is not sufficient to reveal these micro-mechanical fields and therefore requires more physically based constitutive descriptions (Ma et al., 2006a, b; Raabe et al., 2004). The impact of these local changes on bulk texture, grain structure, and stress-strain evolution can then be predicted.

Several versions of DD CPFE models currently exist in literature. Among the most promising are the versions that include not only statistical but also geometrically necessary dislocations and therefore rendering the models size sensitive (Evers et al., 2004; Ma et al., 2006a, b, c) and those that consider individual kinetics of screw and edge dislocations and therefore enabling understanding of phenomena associated with the spread of screw dislocation cores (Alankar et al., 2011; Alankar et al., 2014; Ma et al., 2007). A unique feature of the present model is the consideration of hardening by accumulation of substructure dislocation density, which is desirable for simulating severe plastic strains.

The focus application of the present multi-scale 3D DD-CPFE model is the large-strain rolling deformation of a Zr/Nb lamellar composite at room temperature recently reported in (Knezevic et al., 2014b). As individual single-phase metals, the hcp metal Zr and the bcc metal Nb deform using multiple slip families: \{\overline{1}00\}\{\overline{1}\overline{1}20\}, prismatic slip; \{0001\}\{11\overline{2}0\}, basal slip; and \{10\overline{1}1\}\{\overline{1}\overline{1}23\}, pyramidal slip for Zr and \{110\}\{111\} and \{112\}\{111\} slip in Nb. In
particular, a large amount of research has recently been dedicated to understanding deformation mechanisms in Zr, such as the activation of multiple slip and twinning during large strain processing (Jiang et al., 2008; Knezevic et al., 2013b; Long et al., 2013; Yapici et al., 2009; Zhilyaev et al., 2010), twin nucleation (Beyerlein et al., 2011b; Niezgoda et al.), detwinning (Proust et al., 2010), and slip-twin interactions in abrupt path changes (Capolungo et al., 2009a). These studies established that while the easiest slip mode is prismatic slip, other slip modes, such as pyramidal slip and even basal slip can be activated in large strain deformation (Knezevic et al., 2013b; Long et al., 2013; Yapici et al., 2009). They also show that twinning becomes more prominent below room temperature (Capolungo et al., 2009a) and thus is likely not to be prevalent in the present application. Likewise in Nb, the active slip systems and dislocation dynamics have also been of interest due to its complexity, such as non-Schmid effects (Gröger et al., 2008; Lim et al., 2013; Wang and Beyerlein, 2011), kinematics of glide associated with screw dislocation core structure (Ma et al., 2007), and twinning under shock compression (Gray III, 2012; Zhang et al., 2011). Based on the above studies, it is clear that the large-strain deformation behavior and dislocation-based mechanisms operating within a composite of these two relatively complex metals are expected to be both unusual and interesting.

1.2 Scope of article

This article is structured as follows. We first present the multiscale DD-CPFE modeling methodology, highlighting new features such as the methods needed to incorporate dislocation evolution at the sub-crystalline scale into the CPFE code and to enable modeling severe plastic strains (> 1). Next we use the model to study and predict microstructural evolution of a two-phase hcp Zr/bcc Nb composite in rolling reported previously (Knezevic et al., 2014b). For completeness, we review the experimental results and then describe our independent procedure
for characterizing the DD model parameters for Zr and for Nb using uniaxial compression tests on these materials in monolithic form. The DD-CPFE is then applied to predict texture evolution of the Zr and Nb phases within the composite during large-strain plane strain compression. We show good agreement with the experimental data on texture. Next, we use the model to predict the associated slip activities within the grains and to identify possible gradients in texture due to the bimetal interface. We show that even at large strains, the predicted textures agreed well with the measured deformation textures for each phase in the composite. Also, in spite of large strain development, the texture within the fine lamellar layer thickness (4 µm) was the same as the texture in close proximity of the interfaces. The model predicts that the observed textures developed by a combination of prismatic \langle a \rangle slip, pyramidal \langle c + a \rangle slip, and anomalously basal \langle a \rangle slip in Zr and primarily \{110\}(111) slip and secondly \{112\}(111) slip in Nb.

2. Multiscale modeling approach

The multi-scale model developed here couples self-consistently a 3D crystal plasticity finite element model of a meshed polycrystal, an anisotropic elasticity and rate- and temperature-dependent plasticity formulation for the plasticity of the single crystals, and a dislocation density model for the behavior of individual slip systems within a crystal. Figure 1 presents a flow chart, which illustrates how the different modeling components are connected. To model very large plastic strains encountered during accumulative roll bonding (ARB), we pass important state variables, such as dislocation density and crystallographic orientation from the deformed (old) mesh to the undeformed (new) mesh. Below we describe each modeling component in turn.
2.1 FE homogenization over grains

The overall response of the polycrystal is obtained by the micromechanical finite element model. In this approach, a finite element mesh contains finite elements representing the polycrystal, and each integration point in a finite element of this mesh is associated with a specific crystal lattice orientation. As a platform to integrate our DD hardening law we use the ABAQUS user material subroutine. The single-crystal constitutive model described in the subsequent section operates at each integration point of the finite element mesh. Note that the micromechanical finite element models satisfy equilibrium and compatibility conditions between the grains in the weak numerical sense, and thereby aim to capture more realistically the true interactions between the constituent grains. For each element, the linearized governing FE equation based on the principle of virtual work is shown in the Fig. 1. The left-hand side consists of the FE strain-displacement matrix, \( \mathbf{B} \), material Jacobian, \( \mathbf{J} \), and displacement increment solution field \( \Delta \mathbf{U} \) while the right-hand side represents the residue that includes the Cauchy stress, \( \sigma \), and any applied forces, \( \mathbf{R} \), (Bathe, 1996).

**Figure 1** Multiscale modeling framework for linking sub-grain physics of deformation and polycrystalline response.
Note that from an FE code, a range of information including the deformation gradient $F$ at current, $\tau = t + \Delta t$, and previous, $t$, time increment, time increment $\Delta t$ and a range of material related state variables such as dislocation density and crystal orientation are passed into the material subroutine. The user material model provides the Cauchy stresses, $\sigma$, the Jacobian, $J$, and updated material state variables for each integration point at each time increment.

2.2 Crystal plasticity based constitutive law

We employ a crystal plasticity constitutive law (Kalidindi et al., 1992) to relate material stress to material distortion (stretch plus rotations) at each integration point in the model (Fig. 1). In this law, a material point is allowed to distort by both elastic anisotropy and rate-dependent crystallographic slip. We provide a brief summary below. The reader can find more details in (Kalidindi et al., 1992).

Here we use a finite deformation formulation, in which the total deformation gradient tensor $F$ at a material point can be decomposed into its elastic $F^*$ and plastic $F^p$ components according to

$$ F = F^*F^p $$

where $F^*$ includes the deformation gradients for both elastic stretching and lattice rotation and $F^p$ is the deformation gradient due only to plastic deformation. The following constitutive equation is then used to relate $F^*$ to the stress via (Kalidindi et al., 1992)

$$ T^* = CE^*, \quad T^* = F^{*^{-1}}((detF^*)\sigma)F^{*-T}, \quad E^* = \frac{1}{2}\{F^*T^*F^* - I\}, $$

where $\sigma$ is the Cauchy stress, $T^*$ and $E^*$ are work conjugate stress and strain measures, and $C$ is the fourth-order elasticity tensor. The plastic deformation gradient $F^p$ evolves according to slip at a material point via:

$$ \dot{F}^p = L^p F^p, \quad L^p = \sum_\alpha \dot{\gamma}^\alpha b_\alpha^\alpha \otimes n_\alpha^\alpha, \quad F^p(\tau) = \{I + \Delta tL^p(\tau)\}F^p(t) $$
where $\dot{\gamma}^\alpha$ is the slip rate on $\alpha$, $\mathbf{L}^p$ is the plastic velocity gradient, $\mathbf{I}$ is the identity matrix, and $\mathbf{b}^g_\alpha$ and $\mathbf{n}^g_\alpha$ are the slip direction and the slip plane normal of $\alpha$, respectively, in the undeformed configuration. The $\dot{\gamma}^\alpha$ depends on the resolved shear stress ($\tau^\alpha = \mathbf{T}^* \cdot \mathbf{b}^g_\alpha \otimes \mathbf{n}^g_\alpha$) and the characteristic resistance shear stress ($\tau^\alpha_c$) of $\alpha$, according to the following power-law relationship (Asaro and Needleman, 1985):

$$
\dot{\gamma}^\alpha = \dot{\gamma}_0^\alpha \left( \frac{\tau^\alpha}{\tau^\alpha_c} \right)^m \text{sign}(\tau^\alpha)
$$

(4)

where $\dot{\gamma}_0^\alpha$ is a reference slip rate (taken here as 0.001 s$^{-1}$) and $m$ correlates with the strain rate sensitivity (which is taken here to be 0.01, a value which applies to most metals at low homologous temperatures). The shear rate is used to directly evolve the dislocation density on individual slip systems, as will be explained in the next section.

The lattice spin $\mathbf{W}^*$ can be calculated from $\mathbf{L}^p$ using

$$
\mathbf{W}^* = \mathbf{W}^{app} - \mathbf{W}^p, \quad \mathbf{W}^p = \frac{1}{2} \left( \mathbf{L}^p - \mathbf{L}^{p^T} \right)
$$

(5)

where $\mathbf{W}^{app}$ is the spin applied to the polycrystal and $\mathbf{W}^p$ is the plastic spin, which as shown in the equation on the right, is the skew-symmetric component of $\mathbf{L}^p$ (see Eq. (7)).

An iterative Newton-Raphson scheme for the integration of this constitutive model are given in (Kalidindi et al., 1992).

2.3 Dislocation density evolution law

As depicted in Fig. 1, we use a dislocation density based hardening law formulation to calculate the slip resistance $\tau^\alpha_c$ in Eq. (4) of every slip system $\alpha$ in Zr and Nb as a function of strain, temperature, and strain rate (Beyerlein et al., 2011b; Beyerlein and Tomé, 2008). The DD model presents thermally activated rate laws for dislocation density evolution for individual slip systems and expressions to relate them to the slip resistance $\tau^\alpha_c$. Each rate law for a given slip
system and material has its own dependencies on temperature and strain rate. In this section, the formulation is briefly reviewed.

In the model, we make available multiple slip systems for each material to use for deformation. For Zr, we include prismatic, pyramidal and basal slip. Prismatic \{\bar{1}100\}{\{11\bar{2}0\}} slip is the easiest deformation mode and pyramidal \{10\bar{1}1\}{\{\bar{1}\bar{1}23\}} slip relatively harder (Beyerlein and Tomé, 2008; Kaschner et al., 2006; Tomé et al., 1991). Basal slip is traditionally not considered in Zr for small to moderate strains, but it is known to prevail at larger strains (Knezevic et al., 2013b; Long et al., 2013; Yapici et al., 2009). For Nb, we allow for deformation on the sets of \{110\}{\{111\}} and \{112\}{\{111\}} slip systems. The need for employing these two families of slip for capturing the plastic anisotropy of this metal was elucidated by a combined atomic-discrete dislocation simulation (Wang and Beyerlein, 2011). Other numerical simulations and experiments have provided evidence of non-Schmid effects in bcc metals (Gröger et al., 2008; Lim et al., 2013; Wang and Beyerlein, 2011). Here, we neglect these effects for the time being and acknowledge this important behavior as a topic of future work.

Deformation twinning in both metals is possible, but it only pervasive at colder temperatures (Gray III, 2012; Niezgoda et al., in press) than the room temperature conditions being modeled here. In addition, prior experimental characterization of ARB Cu-Nb composites showed that Nb did not twin, even at the finest nanoscale thicknesses (Carpenter et al., 2013). Therefore, we suppress twinning in this work. Texture measurements made on this material, shown later, confirm that twinning did not occur to an extent that affected the bulk texture.

For each slip system \(\alpha\), its slip resistance \(\tau_c^\alpha\) can be expressed as sum of different contributions as follows:

\[
\tau_c^\alpha = \tau_{o,f}^\alpha + \tau_{o,HP}^\alpha + \tau_{f,or}^\alpha + \tau_{sub}^\alpha.
\] (6)
where $\tau_{o,\alpha}^f$ is a friction stress (dependent on the Peierls stress, interstitials, precipitates and the initial content of dislocation density), $\tau_{o,HP}^\alpha$ is a barrier effect term (e.g., from grain boundaries, twin boundaries), and $\tau_{for}^\alpha$ and $\tau_{sub}^\alpha$ are respectively the contributions from dislocation-dislocation interactions within a grain. The former arises from interactions with a spatially random forest of dislocations $\rho_{for}^\alpha$ and the latter from the density associated with a patterned distribution of dislocations $\rho_{sub}$ (cell walls, subboundaries, etc.). Unlike $\tau_{o,\alpha}^f$ and $\tau_{o,HP}^\alpha$, both $\tau_{for}^\alpha$ and $\tau_{sub}^\alpha$ can evolve with strain due to their direct relationship with dislocation densities that are generated in deformation.

We assume that $\tau_{o,HP}^\alpha$ results from the resistance grain boundaries, spaced by an average grain diameter $d_g$, posed on the dislocations. We relate $\tau_{o,HP}^\alpha$ to the average grain size via a Hall-Petch relationship:

$$\tau_{o,HP}^\alpha = \mu H^\alpha \sqrt{\frac{b^\alpha}{d_g}},$$

where $b^\alpha$ is the value of the Burgers vector, $\mu$ is the effective shear modulus, and $H^\alpha$ is the Hall-Petch parameter. The stresses $\tau_{for}^\alpha$ and $\tau_{sub}^\alpha$ increase as dislocation densities $\rho_{for}^\alpha$ and $\rho_{sub}$ (Beyerlein and Tomé, 2008; Madec et al., 2003) increase via:

$$\tau_{for}^\alpha = \chi b^\alpha \mu^\alpha \sqrt{\rho_{for}^\alpha}, \text{ and } \tau_{sub}^\alpha = k_{sub} \mu^\alpha b^\alpha \sqrt{\rho_{sub}} \log \left( \frac{1}{b^\alpha \sqrt{\rho_{sub}}} \right)$$

where $\chi = 0.9$ is a dislocation interaction parameter, $\mu^\alpha$ is the shear modulus and $k_{sub} = 0.086$ is a mathematical parameter that ensures that Eqn (4) recovers the Taylor law at low dislocation densities (Capolungo et al., 2009b). The stored forest density $\rho_{for}^\alpha$ evolves via a competition between the rate of storage and the rate of dynamic recovery:
where $k_1^a$ is a coefficient for the rate of dislocation storage due to statistical trapping of gliding dislocations by the forest of dislocations and $k_2^a$ is the coefficient for the rate of dynamic recovery, which is given by (Beyerlein and Tomé, 2008)

$$k_2^a \frac{k_1^a}{k_1} g^a \left(1 - \frac{kT}{D^a b^3} \ln \left( \frac{\dot{\epsilon}}{\dot{\epsilon}_o} \right) \right).$$  \hspace{1cm} (10)$$

where $k$, $\dot{\epsilon}_o$, $g^a$, and $D^a$ are respectively Boltzmann’s constant, a reference strain rate, effective activation energy, and a drag stress. The activation barrier $g^a$ corresponds to dislocation de-pinning processes, such as dislocation cross slip and climb. Note that the forest dislocation density increment corresponds to the shear increment on the individual slip systems, obtained using Eq. (4) and the time increment.

It has been proposed and suggested via discrete dislocation dynamics simulations that the processes responsible for dynamic recovery are similar to those that lead to the formation of dislocation substructures, patterns of dislocations, such as cell walls and dislocation sheets (Knezevic et al., 2014b). Dislocation interactions can result in the formation of jogs, dipoles, and locks that self-organize under deformation into relatively low-energy structures (Kuhlmann-Wilsdorf, 1989). To represent the connection, the increment in substructure development is made proportional to the rate of dynamic recovery of all active dislocations via:

$$\Delta \rho_{for} = \sum \alpha \sum b^a \frac{\partial \rho_{rem,for}^a}{\partial \gamma^a} \left| \Delta \gamma^a \right|.$$  \hspace{1cm} (11)$$
where $q$ is a coefficient defining the fraction of an $\alpha$-type dislocations that do not annihilate but become substructure. The increment in the substructure dislocation density corresponds to the summation of the shear increments on the individual slip systems.

In the above model, several material parameters are introduced for each slip system $\alpha$ within each material: the Peierls stress $\tau_{\alpha,f}^\sigma$, trapping rate coefficient $k_1^\sigma$, activation barrier for depinning $g^\sigma$, and drag stress $D^\sigma$. In prior works (Knezevic et al., 2013b), these parameters were characterized for the same three slip modes in Zr and two slip modes in Nb we will consider here. In this work, we will take the opportunity to slightly refine these parameters using the multiscale modeling framework developed here. The independent procedures for parameter characterization and the list of parameters will be presented shortly after presentation of the experimental results, which appears next in Section 3.

2.4 A modification of the analytical CPFE Jacobian matrix

The Jacobian matrix plays a critical role in the rate of global convergence of the FE governing equation, which is based on satisfying global equilibrium (Bathe, 1996). It is defined as $\left(\frac{\partial \sigma}{\partial \Delta \mathbf{E}}\right)$, where $\Delta \mathbf{E}$ is the logarithmic strain increment tensor provided by ABAQUS. The Jacobian matrix is used in Newton-type implicit FE iterations for revising the deformation field at each FE integration point ($\mathbf{F}$) in the current strain increment until the current stress ($\sigma$) satisfies the principle of virtual work. An analytical Jacobian matrix has been rigorously derived and used in a number of standard CPFE codes (Anand, 2004; Delannay et al., 2003; Roters et al., 2010) that predominately use saturation hardening laws of Voce-type. To accommodate the new dislocation density (DD) based hardening law introduced in the previous section, we had to
modify the currently used Jacobian matrix. The required modification pertains to the relationship between $\tau_{c}^{\alpha}$ and $\Delta \gamma^{\alpha}$. Equation (12) shows the modification in terms of $\frac{\partial \tau_{c}^{\alpha}}{\partial \Delta \gamma^{\alpha}}$:

$$d\tau_{c}^{\alpha} = \frac{\partial \tau_{c}^{\alpha}}{\partial \Delta \gamma^{\alpha}} d\Delta \gamma^{\alpha} = \frac{\partial \tau_{f}^{\alpha}}{\partial \Delta \gamma^{\alpha}} d\Delta \gamma^{\alpha} + \frac{\partial \tau_{sub}^{\alpha}}{\partial \Delta \gamma^{\alpha}} d\Delta \gamma^{\alpha}$$

$$d\tau_{c}^{\alpha} = \frac{1}{2} b^{\alpha} \mu^{\alpha} \left[ \chi \left( k_{1}^{\alpha} - k_{2}^{\alpha} \sqrt{\rho_{f,or}^{\alpha}} \right) + k_{sub}^{\alpha} b^{\alpha} \rho_{f,or}^{\alpha} \left[ \ln \left( \frac{1}{b^{\alpha} \sqrt{\rho_{sub}}} \right) - \frac{1}{\ln 10} \right] \right] d\Delta \gamma^{\alpha} \quad (12)$$

### 3. Materials and experiments

To demonstrate the capabilities of the multiscale model described above, we examine texture and microstructural evolution within a two-phase Zr/Nb composite deformed in rolling. In prior work (Knezevic et al., 2014b), this layered composite was fabricated by accumulative roll bonding (ARB) to a final nominal layer thickness of ~4 μm, requiring strains of ~ 4.0. In this section, we briefly review the material and manufacturing details and the experimental results on texture evolution that we aim to predict and refer the reader to (Knezevic et al., 2014b) for more details.

#### 3.1 Materials: Zr and Nb

The composites modeled here consisted of high-purity zirconium with a nominal composition of Hf 35, Fe <50, Al <20, V <50, O <50, N <20, C <22, expressed in weight parts per million (Wt. ppm) and reactor-grade high-purity Nb (99.97% pure, ATI-Wah Chang). Figure 2 shows the starting grain microstructure. The Zr material exhibits equiaxed, twin-free grains with an average grain size of about 40 μm. The average grain size in Nb was much larger, approximately 300 μm. Texture measurements indicate that prior to processing, these two materials had initial texture. Since characterization of HCP textures via ODFs is less common, in this paper, we will use pole figures for the presentation of texture so that both the HCP and BCC
phases can be presented in the same way. As seen in Fig. 3, the resulting Zr texture had a strong basal texture slightly tilted towards the transverse direction (TD). The plate of fully annealed Nb exhibited a (111) fiber texture.

![EBSD orientation maps](image)

**Figure 2** EBSD orientation maps showing the initial microstructure of the as-annealed sample of rolled Zr and Nb. The colors in the orientation maps indicate the orientation of the ND sample direction with respect to the grain orientations (Knezevic et al., 2014b).

![Pole figures](image)

**Figure 3** Pole figures showing the initial texture in the as-annealed sample of rolled Zr and Nb (Knezevic et al., 2014b).
3.2 Accumulative roll bonding of Zr/Nb lamellar composites

Using accumulative roll bonding (ARB) Zr/Nb lamellar composites with individual layer thicknesses ranging from one-millimeter to four microns were successfully fabricated at room temperature (Knezevic et al., 2014b). Optical micrographs of the Zr/Nb layered microstructures deformed to strains of 1.0, 1.5 and 2.0 are shown in Fig. 4.

![Optical micrographs of Zr/Nb composite](image)

**Figure 4** Optical micrographs showing the lamellar microstructures in the Zr/Nb composite produced by the ARB process to layer thicknesses corresponding to the following approximate strain levels/number of layers/average layer thicknesses in µm: 1.0/4/210, 1.5/8/105, 2.0/16/58 (Knezevic et al., 2014b).

3.3 Deformation textures of ARB Zr/Nb composites

The textures of these samples were measured via electron backscattered diffraction (EBSD). These measurements were taken using an FEI XL30 SEM with a TSL/EDAX EBSD camera and software and included data from sufficiently large areas of the material. The textures of the Zr and Nb phases within the composites at various levels of strain (1.0, 1.5, 2.0, 2.5, and 3.5) are given in Figs. 5 and 6 (Knezevic et al., 2014b). Comparisons with the initial texture indicate that the textures have evolved substantially. By strains of 2, the textures have saturated, meaning they did not evolve with further straining.

In many ways, the saturated textures of the phases resemble those of severely rolled monolithic Zr and Nb. For the Zr phase, we observe that the (0002) texture component has spread towards the TD direction along ND-RD plane and concentrated around 30-50° from the
ND direction. The \((10\overline{1}0)\) components have aligned with the RD and concentrated about 30° from the TD and 60° from the RD directions. Last, the \((11\overline{2}0)\) pole has spread towards the RD direction from the ND-TD plane and concentrated at 50° towards the TD direction along the ND-RD plane. These features are consistent with the primary texture components reported previously for Zr (Jiang et al., 2008; Jiang et al., 2007; Linga Murty and Charit, 2006; Philippe, 1994; Philippe et al., 1995; Zhu et al., 2005). For the Nb phase, we see that the deformation textures exhibit typical bcc rolling textures described by the \((001)\) \(\alpha\)-fiber and \((111)\) \(\gamma\)-fiber. These measurements for the composite compare well with previous measurements for single-phase Nb (Ito et al., 2011; Jiang et al., 2006) (Chandra et al., 2007; Heringhaus et al., 1994; Raabe and Lucke, 1994; Vishwanadh et al., 2013). It is worth noting that they also agree with textures of the Nb phase within ARB Cu/Nb composites with micron-thick Nb layers (Carpenter et al., 2012a; Hansen et al., 2013). However, when the Nb phase in a Cu/Nb composite is refined to submicron and nanoscales, the Nb textures are reported to deviate from these typical rolling textures (Carpenter et al., 2012a; Raabe et al., 1992; Raabe et al., 1995). For instance the Nb phase in the cast Cu-20%Nb composite rolled to large strains shows a peak at the \(\{001\}\langle110\rangle\) and a steadily increasing \(\{111\}\langle110\rangle\) component (Raabe et al., 1992; Raabe et al., 1995). In ARB Cu/Nb nanocomposites fabricated via extremely large strains, the Nb phase achieves an extraordinarily sharp texture with components spread between the \(\{112\}\langle110\rangle\) and \(\{113\}\langle110\rangle\) (Carpenter et al., 2012a; Zheng et al., 2013).
Figure 5 Measured pole figures showing the texture evolution in the Zr phase during ARB at strains levels of (a) \(\varepsilon \approx 1.0\), (b) \(\varepsilon \approx 1.5\), (c) \(\varepsilon \approx 2.0\), (d) \(\varepsilon \approx 2.5\) (e) \(\varepsilon \approx 3.5\) (Knezevic et al., 2014b).

Figure 6 Measured pole figures showing the texture evolution in the Nb phase during ARB at strains levels of (a) \(\varepsilon \approx 1.5\), (b) \(\varepsilon \approx 2.0\), (c) \(\varepsilon \approx 2.5\) and (d) \(\varepsilon \approx 3.5\) (Knezevic et al., 2014b).

4. Model characterization

Before predicting the behavior of the Zr/Nb composite in rolling deformation, the material parameters associated with the DD model of Zr and Nb had to be characterized. To do this,
separate simulations and experiments were carried out for uniaxial compression of monolithic Zr and Nb. In simulation, the initial model microstructure consisted of a single-phase polycrystal with 15,000 grain orientations representing the measured initial texture (Fig. 3), and spherical shaped grain. With respect to the coordinate system of the initial texture (Fig. 3), the model material was strained in axial compression in 0.001 strain increments along the ND sample direction, while enforcing zero average stress in the two lateral directions (TD and RD). Figure 7 compares the measured and simulated curves. Apart from small differences in the initial stage of straining Nb, the agreement is good, particularly in the large-strain regime of interest (> 0.5). To achieve this excellent consistency, we only had to make minor adjustments to the DD material parameters for Zr and Nb reported earlier (Knezevic et al., 2013b; Knezevic et al., 2014b). A summary of these parameters are provided in Tables I and II.

![Figure 7 Stress-strain responses of monolithic Zr and Nb in simple compression at room temperature and quasi-static strain rate.](image-url)
Table 1 Constitutive parameters for evolution of slip resistance in the Zr phase

<table>
<thead>
<tr>
<th>α – slip mode</th>
<th>prismatic slip</th>
<th>basal slip</th>
<th>pyramidal slip</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_{o,f}^\alpha$ [MPa]</td>
<td>5</td>
<td>130</td>
<td>105</td>
</tr>
<tr>
<td>$k_1^\alpha$ [m(^{-1})]</td>
<td>3x10(^7)</td>
<td>1x10(^{10})</td>
<td>4x10(^7)</td>
</tr>
<tr>
<td>$g^\alpha$</td>
<td>3.75x10(^{-3})</td>
<td>3.7x10(^{-2})</td>
<td>2.8x10(^{-2})</td>
</tr>
<tr>
<td>$D^\alpha$ [MPa]</td>
<td>330</td>
<td>300</td>
<td>100</td>
</tr>
<tr>
<td>$q^\alpha$ [MPa]</td>
<td>88</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$H^\alpha$ [MPa]</td>
<td>100</td>
<td>100</td>
<td>170</td>
</tr>
</tbody>
</table>

Table 2 Constitutive parameters for evolution of slip resistance in the Nb phase

<table>
<thead>
<tr>
<th>α – slip mode</th>
<th>{110} &amp; {112} slip</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_{o,f}^\alpha$ [MPa]</td>
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</tr>
<tr>
<td>$k_1^\alpha$ [m(^{-1})]</td>
<td>5.2x10(^7)</td>
</tr>
<tr>
<td>$g^\alpha$</td>
<td>3.5x10(^{-2})</td>
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<tr>
<td>$D^\alpha$ [MPa]</td>
<td>230</td>
</tr>
<tr>
<td>$q^\alpha$ [MPa]</td>
<td>14</td>
</tr>
<tr>
<td>$H^\alpha$ [MPa]</td>
<td>50</td>
</tr>
</tbody>
</table>

5. Model set up

Figure 8 shows the 3D bi-phase FE models in the global 1-2-3 (RD-TD-ND) orthogonal coordinate system. The top polycrystalline layer is Nb and the bottom one is Zr. In developing the initial model microstructure, our objective was to have as many elements as necessary to realistically capture the measured initial texture. The elements were hexahedral (brick) elements, containing 8 integration points representing 8 grains with distinct orientations. Each phase has 16x16x8 elements yielding a total of 16x16x16 elements. The total number of crystal
orientations is 32768. In addition, the simulations were carried out for two different realizations, differing only in the assignment of crystallographic grain orientations from the initial measured texture. For the purpose of our present application of predicting and analyzing texture evolution during large plastic co-deformation of the two phases, we averaged texture from both arrangements.

The interface between Zr and Nb was assumed flat at the beginning of each pass. The grains on either side of the Zr/Nb interfaces were kinematically constrained to maintain displacement and traction continuity with all their nearest neighboring grains.

The 3D bi-material polycrystal was deformed in plane strain compression (PSC), an idealization of rolling. This condition best applies to the material in the geometric center of the ARB plate, far from where forward and backward shears can take place at the interface between the sample surface and the rolls. In PSC, the bi-material is compressed in the normal direction, stretched in the rolling direction and constrained from deformation in the transverse direction. Using the global 1-2-3 (RD-TD-ND) orthogonal coordinate system shown in Fig. 8, the velocity gradient tensor associated with PSC was applied:

\[
L_{psc} = \begin{bmatrix}
\dot{\epsilon} & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & -\dot{\epsilon}
\end{bmatrix}
\]  

(13)

The deformation was driven by imposing displacement to all nodes on the top in the negative 3-direction. The imposed strain rate is 0.001/s. The strain increments ranged from 0.005 to 0.01. Nodes in the bottom face were constrained in the 3-direction (ND). Nodes on the front and back faces with normals in the negative 2- and 2-directions, respectively, were constrained in the 2-direction (TD). The right face with normal in the 1-direction was free (rolling direction RD) and the left face was constrained in the 1-direction.
To simulate large strain behavior involved in repeated roll-bonding, the final texture and dislocation density from the previous rolling pass is used to initialize the next rolling pass. The pass strain level followed the experimental schedule where the first pass went up to a strain of 1.0 and every subsequent pass went to a strain of 0.5.

6. Results

6.1 Von Mises and equivalent strain distributions

Figure 8 shows the predicted von Mises stress fields in the deformed bi-phase composite at different stages of straining. It can be seen that the Zr phase experiences higher stress than the Nb phase during co-deformation. This can be expected since in monolithic form, the flow stress of Zr is higher than Nb, as seen in Fig. 7. Figure 9 shows the corresponding equivalent strain fields. Some degree of localization can be seen, starting at the end of the second pass. This strain is approximately the same strain at which shear bands started to form in the experiment (Knezevic et al., 2014b). The other realizations showed similar trends as those seen here.

Figure 8 Initial FE mesh and deformed FE models of the Zr/Nb composite showing Von Mises contours at strain levels indicated in the figures.
Figure 9 Deformed FE models of the Zr/Nb composite showing equivalent strain contours at strain levels indicated in the figures.

6.2 Texture evolution

Figures 10 and 11 show the predicted texture evolution at different rolling reductions with the model predictions for the same strain levels. All the predictions used the same material parameters reported in Tables I and II. As shown, the calculated textures agree well with these measurements. Notably the intensity of the model textures is also consistent with that of the measurement. Typically mean-field techniques, which do not capture the constraints of local grain-grain interactions like CPFE, tend to overestimate texture intensity (Van Houtte et al., 2002).
Figure 10 Pole figures showing the predicted texture evolution in the Zr phase during ARB at strains levels of (a) $\varepsilon \approx 1.0$, (b) $\varepsilon \approx 1.5$, (c) $\varepsilon \approx 2.0$, (d) $\varepsilon \approx 2.5$ and (e) $\varepsilon \approx 3.5$.

Figure 11 Pole figures showing the predicted texture evolution in the Nb phase during ARB at strains levels of (a) $\varepsilon \approx 1.5$, (b) $\varepsilon \approx 2.0$, (c) $\varepsilon \approx 2.5$ and (d) $\varepsilon \approx 3.5$.

Therefore, on average, the textures predicted by the model and measured experimentally of the Zr and Nb phases within the composite on average are similar to those of the monolithic metals when rolled alone. Thus based on bulk texture measurements and predictions, one may
conclude that the bimetal interfaces had no effect on texture evolution. Although on average the
texture did not appear to be affected by the interface, the local texture near the bimetal interface
may differ from that away from the bimetal interface. Such a measurement is non-trivial, but
assessable with the present model. Figure 12 shows the texture for only those Zr and Nb grains
joined to the Zr/Nb interface. As shown, the textures are similar, possessing the same peak
components. The textures are, however, more intense than the bulk, which is likely simply due to
the reduced number of grains in this set. This result suggests that texture gradients did not form
though the thickness of the polycrystalline layers.

**Figure 12** Pole figures showing the predicted textures of (a) Zr phase and (b) Nb phase at a
strain of $\varepsilon \approx 3.5$ in the interface region of the composite.

### 6.3 Slip activity

One of the advantages of this model is its ability to predict the type and distribution of slip at
each material point as a function of strain. Figure 13 shows the slip activity averaged over
polycrystalline Zr and Nb. The model indicates that in large-strain deformation (> 1 strain), the
slip activity eventually saturates. Straining in the Zr phase is accommodated primarily by
prismatic slip. After some amount of straining, a non-negligible amount of basal slip becomes
active. Activation of basal slip in large strain deformation has been seen in other deformation
modes (Knezevic et al., 2013b; Long et al., 2013; Yapici et al., 2009). Straining in the Nb phase
is accommodated by $\{110\}$ slip and secondly by $\{112\}$ slip.
7. Discussion

In the experimental community, much progress has been made towards 3D microstructural characterizations of grain size, grain orientation, grain boundary character, and triple junctions (Groeber et al., 2006; Hefferan et al., 2012; Saylor et al., 2004a; Saylor et al., 2004b). In the modeling community, advancements have also been made in establishing relationships between these microscopic features and macroscopic response. However, a complete 4D (3D plus time) understanding of microstructural-property relationships has yet to be attained and is widely acknowledged as a complex, multiscale problem both experimentally and numerically. Development of 3D multi-scale modeling techniques, which could account for the coupled evolution of subgrain dislocation density, grain boundary character, and grain-scale features, such as the one developed here, can help in this endeavor.

In this work, we present a combined dislocation density based crystal plasticity finite element model. There are several advantages of this model. It is a 3D microstructural model that can provide spatially resolved fields of intra-granular and inter-granular displacement, stress, strain, crystal reorientation, and dislocation densities on individual slip systems. With these capabilities,
it enables predictions for the evolution of texture, grain shape, and grain boundary character due to local effects of grain neighborhoods, grain boundaries, and interface boundaries.

To demonstrate the capability of this model, we studied texture development in an hcp Zr/bcc Nb composite during ARB processing. In these conditions, we successfully predict texture evolution and deformation modes in both phases. For even finer layered composites obtained at much higher rolling reductions, the layers may only span one or two grains through-thickness. In these cases, the interface may play a greater role in texture and microstructural evolution. This expectation is based on prior work on Cu/Nb composites that reported deviations from standard single-phase deformation textures for the Cu or Nb phases within cast Cu–20 wt.% Nb composites rolled to reductions of 99.5%, wire-drawn Cu–20 wt.% Nb, to reductions of 99.98%, and ARB Cu/Nb composites to reductions of 99.96% and greater (Carpenter et al., 2012a; Raabe et al., 1992; Raabe et al., 1995; Zheng et al., 2013).

The advantage of the present 3D CPFE model is that potentially strong interface constraint effects can be captured. In this first application of the DD-CPFE model, we did not account for grain morphology for the sake of simplicity. It is well known that changes in grain morphology with deformation can have an influence on plastic anisotropy and localization, particularly in large strain deformation. The present model can be easily extended to account for the evolution of explicit grain shapes for both phases. Last we mention that the present model has yet to be extended to include several important aspects that interface governs, such as the explicit hardening due to dislocation/interface interactions, including possible annihilation, dislocation absorption, dislocation transmission, dislocation nucleation, or dislocation pile ups as well as dislocation motion in confined layers (Beyerlein et al., 2013a; Beyerlein et al., 2013d; Misra et al., 2005).
8. Conclusions

In summary, we present a 3D multiscale model for polycrystalline metals. The model uniquely incorporates a dislocation density-based hardening law for multiple slip modes into a single-crystal plasticity model, which in turn is linked to the polycrystalline response using finite elements. With these components, the model is capable of predicting the coupled evolution of the local stress and strain fields, dislocation density and texture. The model is applied to the challenging problem of a bi-phase Zr/Nb layered composite that is deformed to large strains. Both Zr and Nb are known to deform by multiple slip modes in monolithic form. The model indicates that for the Zr phase within the composite, prismatic slip is predominant, yet some amount of pyramidal and basal slip activate in the later stages of deformation. In the Nb phase, \{110\} and \{112\} slip are both active, with the former providing more accommodation. To our knowledge this is a unique polycrystal model that is able to connect spatially resolved fields of dislocations, stress, strain, and lattice reorientation to microstructural features such as grain (homophase) and bimetal (heterophase) boundaries.

Acknowledgements

MK and MA were supported by the University of New Hampshire faculty startup funds. IJB would like to acknowledge support through a Los Alamos National Laboratory Directed Research and Development (LDRD) project ER20140348.

References


Chapter 3

This chapter was published as: A study of microstructure-driven strain localizations in two-phase polycrystalline HCP/BCC composites using a multi-scale model, Milan Ardeljan, Marko Knezevic, Thomas Nizolek, Irene J. Beyerlein, Nathan A. Mara and Tresa M. Pollok, International Journal of Plasticity, 74, 35-57. My role in preparing this chapter was to develop 3D grain meshing procedure that was used for creation of polycrystalline microstructures. They were used to realistically represent the two-phase Zr/Nb layered composite microstructures that undergo rolling deformation. I performed all the modeling work presented in this chapter, as well as designing and creating all the figures. I also contributed by writing sections in the paper relevant to the newly developed 3D grain meshing procedure and the modeling efforts that were made to capture the role of microstructure in the development of the local strain concentrations during rolling in this type of composite.
A study of microstructure-driven strain localizations in two-phase polycrystalline HCP/BCC composites using a multi-scale model

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Abstract

In this work, we present a 3D microstructure-based, full-field crystal plasticity finite element (CPFE) model using a thermally activated dislocation-density based constitutive description and apply it to study the deformation of a two-phase hexagonal close packed (HCP)-body center cubic (BCC) Zr/Nb composite. The microstructure models were created using a synthetic grain structure builder (DREAM.3D) and a meshing toolset for the 3D network of grains, grain boundaries, and bimetal interfaces. The crystal orientations, grain shapes, and grain sizes for each phase were initialized based on the measured data. With this novel technique, we aspire to couple the evolution of microstructural heterogeneities with the evolution of spatially resolved mechanical fields during the deformation of complex composites. Here, we apply it to understand the role that microstructure plays in the development of local concentrations in strain and strain rate that can trigger plastic instabilities, such as shear banding. Our chief findings are that 1) local areas of relatively high (and relatively very low) strain concentration occur at triple junctions or quadruple points and then connect with straining to create a banded configuration that extends across the polycrystalline layer, 2) this event starts in the Zr phase and not in the Nb phase, and 3) the triggering hot spots in strain occur at junctions that join grains with very dissimilar reorientation propensities and vice versa for cold spots. In order to determine how such influential localizations can be prevented during processing via application of intermediate
annealing treatments, we used the model to also explore the effects of annealing induced changes in accumulated dislocation density, crystallographic texture and grain shape on the development of strain localizations during subsequent deformation. We found that while it is difficult to avoid strain localizations at grain junctions, when provided a microstructure containing a large few grains spanning the thickness, elongated grain shapes, and reduced dislocation density, the linkage of hot spots in the form of a band can be postponed. At the end we show that when an additional softening mechanism is introduced, these localized strain concentration areas can lead to shear bands.

Keywords: C. Crystal plasticity finite element models; A. Dislocations; A. Interfaces; A. Shear banding; B. Accumulative roll bonding

1. Introduction

In recent years, the fabrication of metallic nanolayered composites (MNC) in bulk form has received much attention (Beyerlein et al., 2013a; Beyerlein et al., 2013b; Mara and Beyerlein, 2014). MNCs are conventionally defined as materials consisting of two or more dissimilar metals, where the smallest dimension of the phases is less than 100 nm. The term bulk is intended to imply that the geometries and quantities have the potential to create structures. In contrast with thin film nanolaminates, these bulk materials are suitable for a wide range of structural applications. Manufacturing bulk MNCs usually involves employing a severe plastic deformation technique, such as equal channel angular extrusion, wire drawing and bundling, and accumulative roll bonding (ARB). These processes refine the initially coarse-structured metals to nano-structured metals without changing the original (bulk) dimensions of the sample (del Valle et al., 2005; Estrin and Vinogradov, 2013; Han et al., 1998; Jahedi et al., 2015a; Jahedi et al., 2015b; Jahedi et al., 2014; Komura et al., 1999; Manna et al., 2002; Saito et al., 1999; Valiev,
2004; Valiev and Langdon, 2006; Wu et al., 2001; Xue et al., 2007). The final sample forms include sheets, plates, rods, or wires.

Other ways of making MNCs include near-equilibrium thermodynamic processes, such as deposition techniques and solidification, but these methods do not make material in bulk (Broussard et al., 1984; Ham and Zhang, 2011; Hannink and Hill, 2006; Misra and Kung, 2001). Nonetheless, through studying the MNCs made in this fashion, a basic understanding of MNC properties has been developed. Most notably, from studies of nanolayered films made by physical vapor deposition (PVD), they have proven to possess exceptional properties, such as strengths over 5 to 10 times that of their constituents, hardness values that are several orders of magnitude higher, and microstructural stability in extreme, harsh environments (Beyerlein et al., 2013a; Mara et al., 2008, 2009; Misra et al., 2007; Misra et al., 2004).

Bulk MNCs made via mechanical deformation are not as well understood, since severe plastic deformation processes create microstructures and textures very different from those of PVD MNCs. The severe plastic deformation ARB process mentioned above makes MNCs in sheet form comprised of alternating nanolayers of the two metals (Jiang et al., 2008; Knezevic et al., 2014e; Saito et al., 1999), which is similar to the layered architecture of the deposited nanolayered PVD composites. It was only recently that Cu/Nb MNCs made via ARB, like the PVD Cu/Nb nanolayers, were found to also exhibit outstanding strength (Beyerlein et al., 2013b; Mara and Beyerlein, 2014), hardness (Monclús et al., 2013), ductility (Nizolek et al., 2014), resistance to light-ion radiation (Han et al., 2013), thermal stability (Carpenter et al., 2012; Zheng et al., 2013), and shock resistance (Han et al., 2014). This initial set of findings provides motivation to continue developing bulk MNCs for other material systems.
Using the ARB process, MNCs of many other composite material systems have been made, such as Al/Sc (Quadir et al., 2009), Ag/Fe (Yasuna et al., 2000), Cu/Au (Li et al., 2008), Ag/Ni (Kikuchi et al., 1997), and Cu/Fe (Shingu et al., 2001), Cu/Zr (Ohsaki et al., 2007). However, an important issue encountered in fabricating MNCs via ARB of any given two-phase system is plastic instabilities. The onset of instabilities, such as shear banding, during the ARB process can prevent refinement from coarse (mm to µm) layers to nano layers. For instance, in recent work (Ardeljan et al., 2014b; Carpenter et al., 2015; Carpenter et al., 2014b), multilayered sheets of Zr/Nb system were made via ARB. After large strains of ~4, shear bands initiated and the layers could not be refined below several microns (Fig. 1a). In a second attempt, periodic annealing treatments (575°C for one hour) between ARB rolling passes were introduced, enabling refinement to the same thickness without shear band formation (Fig. 1b). Due to the successfully suppression of shear band formation, material with individual layer thicknesses of ~90 nm was achieved through further processing (Carpenter et al., 2015; Carpenter et al., 2014b).

The reasons that intermediate annealing steps prevented shear banding were not clear. Post-mortem electron backscattered diffraction (EBSD) characterization indicated that, for polycrystalline Zr layers above 1 micron, the grain size and shape and the texture of the Zr phase changed after each annealing step. Further, the EBSD analysis suggested that the intra-granular substructure and stored dislocations changed as a result of intermediate annealing (Carpenter et al., 2014b). The Nb phase, with a much higher melting point, however, experienced no such dramatic changes in microstructure. Evidently one or more of the annealing-induced microstructural changes, whether it is in grain shape, grain size, texture, or stored dislocations, helped to thwart shear band formation. In addition, these changes also change the constitutive behavior of Zr phase and its relative deformation properties with that of the Nb phase in
subsequent deformation. Either of these changes could have also prevented plastic instabilities. From a fundamental viewpoint, it is desirable to identify the basic factors that postponed shear banding with the goal that these insights could enable fabrication of MNCs from a broader set of material systems.

![Figure 1](image)

**Figure 1** Optical micrographs showing lamellar microstructures in the Zr/Nb composite produced by the ARB process: (a) without annealing and (b) with an annealing step after every other ARB pass. Strain levels/number of layers/average layer thicknesses in µm are as follows 2.7/16/127, 3.5/32/58, and 4.1/64/30. The micrographs at 127 and at 30 µm layer thicknesses are shown after the annealing step.

Plasticity models can be useful in relating microstructure to plastic deformation properties. Mean-field crystal plasticity models of various sophistication levels ranging from upper bound Taylor type (Taylor, 1938) to self-consistent type (Lebensohn and Tomé, 1993) are capable of predicting the texture development and offering insights into the active deformation mechanisms. These are well established in literature with numerous applications in predicting monotonic deformations as standalone codes (Al-Harbi et al., 2010; Fast et al., 2008; Fromm et al., 2009; Kalidindi et al., 2009; Knezevic et al., 2009; Knezevic et al., 2014b; Knezevic and Kalidindi, 2007; Knezevic et al., 2008a; Knezevic and Landry, 2015; Knezevic and Savage, 2014; Shaffer
et al., 2010; Van Houtte, 1982; Van Houtte et al., 2002; Wu et al., 2007) or non-monotonic within finite elements (Barton et al., 2008; Beaudoin et al., 1993; Knezevic et al., 2014d; Knezevic et al., 2013c; Knezevic et al., 2013d; Knezevic et al., 2012b; Zecevic et al., 2015b, c). However, they cannot treat localizations and inhomogeneous deformation. Relating microstructural features to mechanically induced localizations requires full-field, spatially resolved crystal plasticity techniques. Many of these have been developed in recent years, such as crystal plasticity finite element (CPFE) (Knezevic et al., 2014c; Knezevic et al., 2010; Roters et al., 2010) and Green’s function based FFT (Lebensohn et al., 2012). Further, to understand how details of grain structure, texture, and hardening can lead to the development of localized strains and stresses, these techniques must employ physically based laws for dislocation slip (Ardeljan et al., 2014a; Keshavarz and Ghosh, 2013; Ma et al., 2006, 2007) and experimentally motivated or informed 3D microstructures (Knezevic et al., 2014c).

1.1 Objectives

In this work we 1) integrate a 3D microstructure based, multi-scale crystal plasticity finite element (CPFE) modeling tools, 2) apply these to understand the relationship between microstructure and strain localizations during plane strain compression, and 3) study the effect of changes in dislocation density, texture, and grain shape and size induced by annealing on the tendency to generate local strain concentrations. Experimentally informed representations of the deformed or annealed polycrystalline grain structures within Zr/Nb micron-layered composites are constructed in DREAM.3D. Then, as a separate procedure, the grains and grain boundaries in these microstructure models are meshed. The CPFE constitutive model uses a hardening law based on dislocation density evolution to dictate slip. In the hardening law, the dislocation densities for each of the three modes of slip in Zr (〈a〉 prismatic, 〈c+a〉 pyramidal, and 〈a〉
basal) and two modes of slip in Nb (\(
\{\overline{1}0\}\{111\} \) and \(\{\overline{1}12\}\{111\}\)) evolve with their own individual dependencies on strain, temperature and strain rate. Using this multi-scale model, simulations of plane strain compression are carried out to investigate the connection between microstructural evolution and the onset of strain localizations in 3D. We find that the more intense spots of strain concentration (hot spots) begin in the Zr phase and not in the Nb phase. They form first at points where three or more grains meet (i.e., triple junctions, quadruple points) at low strains and then bands of strain concentration form that connect these hot spots across grains with continued straining. These hot spots are rare and occasional considering the large number of grain junctions within the grain boundary network of the model. One of our chief findings is that such triggering hot spots in strain occur at junctions that join grains with very dissimilar reorientation propensities and vice versa for cold spots.

1.2 Background

The development of microstructural instabilities in polycrystalline metals during mechanical deformation involves many physical changes occurring at different length scales. One example of a grain-scale manifestation of such changes is the generation of localized strain concentrations and subsequent shear band formation (Dodd and Bai, 2012; Meyers, 1994; Wright, 2002). Shear bands are narrow regions of highly localized strains or strain rates and due to the rapid rates of deformation can experience significant increases in temperature. Shear band formation and its underlying mechanisms have been thoroughly studied over the past decades. It has been shown that crystallographic orientation, grain morphology, and microstructure evolution can influence the formation of shear bands (Anand and Kalidindi, 1994; Antolovich and Armstrong, 2014; Wagner et al., 1995).
Shear bands in FCC metals have been the focus of many of these studies. In FCC metals with medium and high stacking fault energy, such as Al and Cu, work/thermal softening followed by mechanisms of dynamic recovery and recrystallization in localized regions are believed to cause strain localization and subsequent shear band formation (Hines and Vecchio, 1997; Meyers et al., 2002). In this case, localized deformation occurs when the loss of strength from work softening processes becomes greater than the increase in strength due to work hardening. In low stacking fault energy face-centered cubic (FCC) metals, such as alpha brass, the mechanisms underlying shear band formation are believed to be controlled by deformation twinning (Duggan et al., 1978). Similarly, in HCP metals that can twin easily, it was found that when the twinning capacity became exhausted and significant work hardening due to slip-twinning interactions is achieved, massive shear band formation and large strain localizations occur (Al-Samman and Gottstein, 2008).

To better understand the deformation characteristics involved in shear banding, the microstructure within the band has been evaluated. Several experimental studies have shown that depending on the level of strain achieved within the shear bands, the strain rate of the shear band deformation, and the material studied, the grain structure within the shear bands can range from highly elongated subgrains, to fragmented subgrains possessing a high degree of misorientation, to small recrystallized grains. In some BCC metals, such as interstitial-free steel (Lins et al., 2007), dynamic recrystallization was found to operate within the shear bands. In others, such as in Ta, Nb and Ta-10W alloys, no evidence of recrystallization was found but only significant grain elongation and dynamic recovery (Nemat-Nasser and Guo, 2000; Pérez-Prado et al., 2001). In these cases, the temperature rise associated with deformation in the localized regions of shear bands was insufficient to achieve dynamic recrystallization. Evolution of microstructure inside
the shear bands in nanograined Fe has been studied (Wei et al., 2002). The study revealed that
the microstructure inside the shear bands has large dislocation density and that geometric
softening rather than adiabatic softening is the origin for the inhomogeneous deformation. The
ultrafine size grains make it possible for a large group of grains to quickly develop the texture
favorable for slip propagation in a cooperative manner, facilitating the localization of the plastic
deformation.

Significantly less well studied are localized regions of high strain or stress in two-phase
lamellar composites where not only the constituents but also the co-deformation constraints
between the phases are expected to influence their development. Under rolling, the differences in
yield strength and hardening behavior between the two metals and characteristics of the bimetal
interface have been found to be important (Jia et al., 2013; Mara et al., 2010; Quadir et al., 2009;
Steif, 1987). Using TEM analyses, it was shown that the crystallographic character of the bimetal
interface could also influence the formation of shear bands (Zheng et al., 2014).

Since kinetics of diffusion-based recrystallization models were found unable to explain the
formation of subgrains due to the speed of formation within shear bands (estimated to be
between 10 and 50 μs), ideas based on crystal plasticity have been offered. One of which is a
‘progressive subgrain misorientation (PrisM) recrystallization’ aimed at capturing the
mechanically driven subgrain reorientation without any recrystallization kinetics (Hines et al.,
1998). It was proposed that mechanisms termed as ‘Rotational Dynamic Recrystallization’
operate within shear bands (Meyers et al., 2001; Meyers et al., 2002). Modeling of shear band
formation in brass has been accomplished by modifying the shear components of the velocity
gradient corresponding to shear bands in grains that had accumulated a substantial twin volume
fraction (Kalidindi, 2001). Likewise, introducing explicit non-crystallographic shear banding
mechanisms has also been successful in capturing shear band formation (Anand and Su, 2005; Jia et al., 2012a; Jia et al., 2012b). This approach was found to help weaken certain texture components, such as the Copper and S, and strengthen the Brass texture component responsible for localizations.

Very recently, CPFE has been applied to simulate two-phase lamellar FCC/FCC and FCC/BCC composites (Hansen et al., 2013; Jia et al., 2013; Mayeur et al., 2015; Mayeur et al., 2013) and HCP/BCC composites (Ardeljan et al., 2014a) under plane strain compression. In these models, the individual phases were either polycrystalline or single crystals and in all cases, assumed to co-deform at the bimetal interface. In the polycrystalline models, localized areas of stress or strain concentrations were observed. In the bicrystal models, whether localizations developed depended on the particular orientations being coupled (Jia et al., 2013; Mayeur et al., 2013) and how much the interface influenced slip (Mayeur et al., 2015). Simulating the transition from localized stress or strain to shear banding, however, required incorporating an additional, non-crystallographic shear band system (Jia et al., 2013).

2. Experimental materials and methods

Before developing the multi-scale model, we first describe briefly, the experiment that motivated this work. Much of the material microstructure, texture, and constitutive response will be used to define the starting microstructures and material properties used in the model.

2.1 Materials: Zr and Nb

The composites modeled here consisted of high-purity Zr with a nominal composition of Hf 35, Fe <50, Al <20, V <50, O <50, N <20, C <22, expressed in weight parts per million (Wt. ppm) and reactor-grade high-purity Nb (99.97% pure, ATI-Wah Chang).
Both materials were processed into 1 mm thick plates. The textures in the starting plates have been reported in prior papers (Ardeljan et al., 2014a; Knezevic et al., 2014e). For completeness of the present study, we show the starting textures in Fig 2a. The plate of fully annealed Nb (at 950 °C for 1h) exhibited a (111) fiber texture. The plate of Zr had a strong basal texture slightly tilted towards the transverse direction (TD) that resulted from a series of processing steps: first upset forging; next, clock-rolling and annealed at 550°C for 1h; and last, right before ARB processing, straight rolling and annealing at 600°C for 1h.

Figure 2 also compares the stress-strain response of the monolithic Zr and Nb in thru-thickness compression (Ardeljan et al., 2014a). As shown, for the room temperature and low strain rate conditions, these two metals do not differ appreciably in their flow response.

2.2 Accumulative roll bonding of Zr/Nb lamellar composites

In prior work, Zr/Nb multilayer composites were processed with and without periodic annealing treatments (575°C for one hour) between roll bonding steps. The evolution of crystallographic texture after roll bonding of the composites was measured using both neutron
diffraction (Carpenter et al., 2014b) and electron backscattered diffraction (EBSD) (Ardeljan et al., 2014a; Knezevic et al., 2014e). Neutron diffraction was performed using the HIPPO spectrometer at the Los Alamos Neutron Science Center (LANSCE) (Bourke et al., 2002). EBSD was performed on an FEI XL30 SEM using a TSL/EDAX EBSD camera and software.

Without intermediate annealing, fine shear bands appeared after large rolling reductions at a strain of approximately 4.0 (Knezevic et al., 2014e) (Fig. 1a). With intermediate annealing, shear banding was postponed and layer refinement to the nanoscale was possible (Carpenter et al., 2014b). The layer thickness at which shear bands were first noticed was about 30 µm, where multiple grains still span the Zr and Nb layers. Thus, the material that we wish to analyze is a multilayer composite consisting of polycrystalline layers containing submicron grains.

To elucidate the role of microstructure evolution on strain localization and eventual shear banding, the texture and the polycrystalline microstructures of both the Zr and Nb phase at a strain of 2.7 after annealing were used to initialize the model. Figure 3 shows measured texture at the strain of 2.7 and the corresponding reduced texture used to assign the initial texture in the simulations. Then the model two-phase layered material was rolled to additional strains of 1.0 to 1.4, giving a total of 3.7 to 4.1, which is the range of strain where the onset of shear banding was seen.
Figure 3 Pole figures showing initial texture in the annealed sample of ARB processed Zr/Nb to a layer thickness of 127 µm (a) measured textures using neutron diffraction for Zr and EBSD for Nb and (b) corresponding textures used in simulations (represented using 981 weighted orientations for Zr and 165 orientations for Nb).

3. Multi-scale modeling approach

The present work integrates a set of existing computational models to study two-phase composites. To best capture the effects of orientation, orientation gradients near grain boundaries, grain shape, and grain neighbor interactions on strain concentrations, we employ a 3D CPFE framework combined with experimentally informed models for the grain microstructures. The latter are generated in DREAM.3D (2013b). Output from DREAM.3D in the form of grain boundary surface/shell mesh is imported into a tool set, which we have recently built (Knezevic et al., 2014c) for creating solid 3D meshes for CPFE calculations.

The grains, both after rolling and before and after annealing steps, range from elongated to equi-axed and have different sizes in the Zr and Nb phase. We found DREAM.3D to successfully generate synthetic microstructure matching given aspect ratio, size and morphological orientation distributions. Additionally, grain boundary mesh ensures modeling conformal grain boundaries between grains, which is vital. Plastic instabilities and strain
concentrations could form first at grain boundaries or interfaces, and thus, artificially planar (non-conformal) boundaries could lead to misleading results. Previously, in a study to understand where voids in microstructures could nucleate, a visco-plastic 3D Fast Fourier Transform (FFT) technique was applied to an FCC polycrystal to study local concentrations in stress (hot spots), and there it was shown that both hot and cold spots were primary generated at grain boundaries, triple junctions, and quadruple points (Rollett et al., 2010) although the FFT technique is unable to model conformal grain boundaries. We expect to observe a similar phenomenon here and thus we aim to accurately represent the boundaries and junctions in the microstructure.

3.1 Grain and grain boundary structure of the Zr/Nb composite

Consistent with the experimental measurements of the annealed grain structure after a strain of 2.7 (Carpenter et al., 2014b), the grain aspect ratios were specified in DREAM.3D using a lognormal grain size distribution with a mean and standard deviation of 4.5 and 0.025 for Zr and 5.1 and 0.025 for Nb. The resulting distributions per phase are shown in Fig. 4c. The distributions were specified for the RD-ND plane together with the grain aspect ratio parameter of eight in the RD. The resulting elongated grain structure consisting of 981 grains in Zr and 165 grains in Nb is shown in Fig. 4a. Starting from the grain surface meshes, described by triangular shell elements, we generated the 3D solid mesh in Patran, the finite element preprocessor from MSC Software (2013d). The grain boundary surface mesh ensures a conformal mesh between neighboring grains. A converter, written in Matlab (2013c), was developed for purposes of post-processing the Patran output files containing the 3D mesh information for each grain. As a final step, this code generates a valid ABAQUS input file (2013a), where each grain is defined as a separate element set. The entire 3D mesh of the grain structure consists of approximately 1,500,000 C3D4 (continuum 3D 4-node) linear tetrahedral elements (Fig. 2b). The same crystal
orientation is assigned to every integration point that belongs to the same element associated with a 3D grain. During the deformation simulation, the crystal orientations evolve at each integration point with strain, allowing for inter- and intra-granular misorientations from the starting state to develop.

A CPFE simulation involving ~1,500,000 linear elements to a strain of 1.4 is computationally very intensive since a set of highly non-linear, extremely stiff, constitutive equations with poor convergence characteristics intrinsic to crystal visco-plasticity theory needs to be solved for each constituent crystal at every integration point at each trial time increment. An earlier study (Knezevic et al., 2014c) revealed that the use of higher order elements, e.g., C3D10M, in place of C3D4 only extends the computation time involved by approximately four times since a C3D10M element has four integration points as opposed to only one per C3D4 element. While the stress-strain fields can be represented with a fewer number of the higher order elements in comparison with the linear elements, the highly irregular geometry of a typical grain structure demands a large number of elements. Therefore computationally less intensive linear elements were selected for the earlier and the present study. The selected element size was based on our earlier work (Knezevic et al., 2014c).
Figure 4 Numerical setup of the 127 µm layered microstructure: (a) two phase synthetic polycrystalline aggregate with 1200 µm in RD, 480 µm in TD and 1320 µm in ND consisting of 3D cubic voxels generated in DREAM.3D, and (b) corresponding mesh of 3D grains consisted of 1.5 million C3D4 (continuum 3D 4-node) tetrahedral elements. (c) Grain size distribution in the RD-ND plane together with the aspect ratio parameter of eight in the RD was set in DREAM.3D to generate grain structure.

3.2 Crystal plasticity based constitutive law

We employ a crystal plasticity constitutive law (Kalidindi et al., 1992; Kalidindi et al., 2006; Knezevic et al., 2008b) to relate material stress to material distortion (stretch plus rotations) at each integration point in the model. In this law, a material point is allowed to distort by both elastic anisotropy and rate-dependent crystallographic slip. This model was developed earlier and details can be found in (Kalidindi et al., 1992). A brief summary is provided below.

Here we use a finite deformation formulation, in which the total deformation gradient tensor $\mathbf{F}$ at a material point can be decomposed into its elastic $\mathbf{F}^*$ and plastic $\mathbf{F}^p$ components according to

$$\mathbf{F} = \mathbf{F}^* \mathbf{F}^p$$ (1)
where \( \mathbf{F}^* \) includes the deformation gradients for both elastic stretching and lattice rotation and \( \mathbf{F}^p \) is the deformation gradient due only to plastic deformation. The following constitutive equation is then used to relate \( \mathbf{F}^* \) to the stress via:

\[
\mathbf{T}^* = \mathbf{CE}^*, \quad \mathbf{T}^* = \mathbf{F}^{-1}[(\det \mathbf{F}) \mathbf{\sigma}] \mathbf{F}^{-T}, \quad \mathbf{E}^* = \frac{1}{2} \{ \mathbf{F}^T \mathbf{F}^* - \mathbf{I} \}
\]

where \( \mathbf{\sigma} \) is the Cauchy stress, \( \mathbf{T}^* \) and \( \mathbf{E}^* \) are work conjugate stress and strain measures, and \( \mathbf{C} \) is the fourth-order elasticity tensor. The plastic deformation gradient \( \mathbf{F}^p \) evolves according to slip at a material point via:

\[
\dot{\mathbf{F}}^p = \mathbf{L}^p \mathbf{F}^p, \quad \mathbf{L}^p = \sum_\alpha \dot{\gamma}^\alpha \mathbf{b}_0^\alpha \otimes \mathbf{n}_0^\alpha
\]

where \( \dot{\gamma}^\alpha \) is the slip rate on \( \alpha \), \( \mathbf{L}^p \) is the plastic velocity gradient, and \( \mathbf{b}_0^\alpha \) and \( \mathbf{n}_0^\alpha \) are the slip direction and the slip plane normal of \( \alpha \), respectively, in the un-deformed configuration. The \( \dot{\gamma}^\alpha \) depends on the resolved shear stress (\( \tau^\alpha = \mathbf{T}^* \cdot \mathbf{b}_0^\alpha \otimes \mathbf{n}_0^\alpha \)) and the slip resistance (\( \tau^\alpha_c \)) of \( \alpha \), according to the following power-law relationship (Asaro and Needleman, 1985; Hutchinson, 1976):

\[
\dot{\gamma}^\alpha = \dot{\gamma}_0^\alpha \left( \frac{\left| \tau^\alpha \right|}{\tau^\alpha_c} \right)^m \text{sign}(\tau^\alpha)
\]

where \( \dot{\gamma}_0^\alpha \) is a reference slip rate (taken here as 0.001 s\(^{-1}\)) and \( m \) correlates with the strain rate sensitivity (which is taken here to be 0.01, a value which applies to most metals at low homologous temperatures).

The lattice spin \( \mathbf{W}^* \) can be calculated from \( \mathbf{L}^p \) using

\[
\mathbf{W}^* = \mathbf{W}^{app} - \mathbf{W}^p, \quad \mathbf{W}^p = \frac{1}{2}(\mathbf{L}^p - \mathbf{L}^{pT})
\]

where \( \mathbf{W}^{app} \) is the spin applied to the polycrystal and \( \mathbf{W}^p \) is the plastic spin, which as shown in the equation on the right, is the skew-symmetric component of \( \mathbf{L}^p \) (see Eq. (3)).

An iterative Newton-Raphson scheme for the integration of this constitutive model are given in (Kalidindi et al., 1992).
3.3 Dislocation density (DD) evolution law

We use dislocation density based (DD) hardening law framework to describe the evolution of slip resistance for slip systems in Zr and Nb as a function of strain, temperature, and strain rate (Beyerlein et al., 2011; Beyerlein and Tomé, 2008; Knezevic et al., 2012a; Knezevic et al., 2013e; Knezevic et al., 2015). Each slip mode \( \alpha \) in Zr and Nb has its own dislocation density evolution law and dependencies on temperature and strain rate. Deformation twinning would follow a completely different nucleation and propagation law (Beyerlein et al., 2011; Lentz et al., 2015a; Lentz et al., 2015b; Niezgoda et al., 2014; Zecevic et al., 2015a) but is not included here since twinning was not observed non-negligible amounts. In this section, the slip hardening formulation is briefly reviewed.

In the model, the slip resistance for all slip modes \( \alpha \), \( \tau_{c \alpha} \), is assumed to have the same basic form:

\[
\tau_{c \alpha} = \tau_{0 \alpha} + \tau_{for \alpha} + \tau_{sub \alpha}
\]  

(6)

The first term on the right hand side of Eq. (7) \( \tau_{0 \alpha} \) is the athermal resistance to slip. It does not evolve with strain and represents the resistance to propagation apart from dislocation interactions. It is given by a sum of a constant friction stress \( \tau_{0, f \alpha} \) and an initial grain-size dependent Hall-Petch contribution \( \tau_{0, HP \alpha} \):

\[
\tau_{0 \alpha} = \tau_{0, f \alpha} + \tau_{0, HP \alpha}
\]  

(7)

The latter is given by:

\[
\tau_{0, HP \alpha} = \mu H^\alpha \sqrt{b_{\alpha}}/d_g
\]  

(8)

where \( b_{\alpha} \) is the value of the Burgers vector corresponding to the \( \alpha \)-slip mode, \( d_g \) is the grain size, \( \mu \) is the effective shear modulus, and \( H^\alpha \) is a Hall-Petch coefficient.
The next two terms in Eq. (7), $\tau^\alpha_{for}$ and $\tau^\alpha_{sub}$, result from dislocation interactions and, unlike the athermal term, evolve with strain. The former $\tau^\alpha_{for}$ results from obstacles of stored ‘forest’ dislocations with density $\rho^\alpha_{for}$ and is related to $\rho^\alpha_{for}$ by a Taylor law:

$$\tau^\alpha_{for} = \chi b^\alpha \mu \sqrt{\rho^\alpha_{for}}$$  \hspace{1cm} (9)

where $\chi$ is a dislocation interaction parameter. As is customary, we choose a common value of 0.9 for $\chi$ (Lavrentev, 1980; Mecking and Kocks, 1981).

The density $\rho^\alpha_{for}$ evolves with slip strain per mode $\gamma^\alpha$ based on the competition between the rate of dislocation storage and dynamic recovery (Kocks and Mecking, 2003):

$$\frac{\partial \rho^\alpha_{for}}{\partial \gamma^\alpha} = k_1^\alpha \sqrt{\rho^\alpha_{for}} - k_2^\alpha (\dot{\gamma} T) \rho^\alpha_{for}$$  \hspace{1cm} (10)

where $k_1^\alpha$ is a rate coefficient associated with storage via statistical trapping of gliding dislocations by forest obstacles and $k_2^\alpha$ is a rate coefficient for dynamic recovery by thermally activated mechanisms (e.g., cross slip) (Beyerlein and Tomé, 2008) given by

$$\frac{k_2^\alpha (\dot{\gamma} T)}{k_1^\alpha} = \frac{\chi b^\alpha}{g^\alpha} \left( 1 - \frac{k T}{D^\alpha (b^\alpha)^3} \ln \left( \frac{\dot{\gamma}}{\dot{\gamma}_0} \right) \right)$$  \hspace{1cm} (11)

where $T$, $\dot{\gamma}$, $k$, $\dot{\gamma}_0$, $g^\alpha$, and $D^\alpha$ are respectively temperature (K), the effective macroscopic strain rate, Boltzman’s constant, a reference effective strain rate, a normalized effective activation enthalpy, and a drag stress.

The last term $\tau^\alpha_{sub}$ is the resistance due to dislocation substructures with density $\rho_{sub}$, which tends to be much larger than $\rho^\alpha_{for}$. Due to the concomitantly smaller dislocation separation distances $\Lambda$ within substructure, such as within cell and lamella walls, the resistance to slip is enhanced, appearing to follow $\sqrt{1/\Lambda \log(\Lambda)}$ (Madec et al., 2003). On this basis, $\tau^\alpha_{sub}$ is related to $\rho_{sub}$ via an extended Taylor law given by:
\[
\tau_{\text{sub}}^\alpha = k_{\text{sub}} \mu b^\alpha \sqrt{\rho_{\text{sub}}} \log \left( \frac{1}{b^\alpha \rho_{\text{sub}}} \right)
\]  
(12)

where \( k_{\text{sub}} = 0.086 \) (Madec et al., 2003), a numerical constant that makes sure that the extended law Eq. (13) converges to the conventional one Eq. (10) when \( \rho_{\text{sub}} \) is sufficiently small\(^1\). Further, the rate of substructure development is coupled to the rate of dynamic recovery of active \( \alpha \)-type slip via:

\[
d\rho_{\text{sub}} = \sum_\alpha q_\alpha b_\alpha \sqrt{\rho_{\text{sub}}} \left[ k_2 \rho_{\text{for}} \right] d\gamma_\alpha
\]  
(13)

where \( q_\alpha \) is a rate coefficient linking the rate of recovery of \( \alpha \)-type dislocations to the rate of substructure development. It can also depend on temperature, strain level, and strain rate (Beyerlein and Tomé, 2008; Knezevic et al., 2013a).

The slip modes made available to Zr are prismatic \( \{1\overline{1}00\} \langle 1\overline{1}20 \rangle \) slip, which is the easiest deformation mode in Zr; pyramidal \( \{10\overline{1}1\} \langle \overline{1}1\overline{2}3 \rangle \) slip, the relatively hard deformation mode; and basal \( \{0001\} \langle 1\overline{1}20 \rangle \) slip, the hardest one.

The slip modes used in Nb are the \( \{1\overline{1}0\} \langle 1\overline{1}1 \rangle \) and \( \{\overline{1}\overline{1}2\} \langle 1\overline{1}1 \rangle \) slip systems, which have been shown in prior modeling works to be important (Bhattacharyya et al., 2015; Ito and Vitek, 2001; Knezevic et al., 2014a; Ma et al., 2007; Wang and Beyerlein, 2011). Deformation twinning in Nb for this strain rate, temperature, and crystal sizes has not been observed and hence is neglected here (Beyerlein et al., 2014).

The hardening parameters associated with the above model for the different slip modes in Zr and Nb have been determined in prior work (Ardeljan et al., 2014a) and are shown in Tables 1

\(^1\) Because Eq. (13) applies to both, large and small values of \( \rho \), it can alternatively be used for both \( \tau_{\text{for}} \) and \( \tau_{\text{sub}} \), as was done in Capolungo, L., Beyerlein, I.J., Tomé, C.N., 2009a. Slip-assisted twin growth in hexagonal close-packed metals. Scripta Materialia 60, 32-25.
and 2. Since the starting material was annealed, the initial dislocation density was set to a small value of $10^{12} \text{ m}^{-2}$, which is typical of annealed materials.

<table>
<thead>
<tr>
<th>$\alpha$ – slip mode</th>
<th>prismatic slip</th>
<th>basal slip</th>
<th>pyramidal slip</th>
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<tr>
<td>$\tau_{0,f}^\alpha$ [MPa]</td>
<td>5</td>
<td>130</td>
<td>105</td>
</tr>
<tr>
<td>$k_1^\alpha$ [m$^{-1}$]</td>
<td>$3 \times 10^7$</td>
<td>$1 \times 10^{10}$</td>
<td>$4 \times 10^7$</td>
</tr>
<tr>
<td>$g^\alpha$</td>
<td>$3.75 \times 10^{-3}$</td>
<td>$3.7 \times 10^{-2}$</td>
<td>$2.8 \times 10^{-2}$</td>
</tr>
<tr>
<td>$D^\alpha$ [MPa]</td>
<td>330</td>
<td>300</td>
<td>100</td>
</tr>
<tr>
<td>$q^\alpha$ [MPa]</td>
<td>88</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$H^\alpha$ [MPa]</td>
<td>100</td>
<td>100</td>
<td>170</td>
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</table>

<table>
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<th>$\alpha$ – slip mode</th>
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<tr>
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<td>$g^\alpha$</td>
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<td>$H^\alpha$ [MPa]</td>
<td>50</td>
</tr>
</tbody>
</table>

3.4 Boundary conditions for rolling simulations

The 3D two-phase microstructure models described above in section 3.1 were deformed in plane strain compression (PSC), an idealization of rolling deformation. PSC conditions are known to be a reasonable assumption for the sheet interior, the material away from the rolls in the through-thickness direction and from the in-plane edges (Kocks et al., 1998). In the middle of
the sheet, the transverse strain is zero and there are no shear components due to the interaction between rolls and the sheet. Under PSC conditions, we are modeling a small volume of the material containing one phase interface. Therefore, the material is constrained by the neighboring material imposing plane strain conditions. The volume is compressed in the normal direction (ND), extended in the rolling direction (RD) and constrained from deforming in the transverse direction (TD). The velocity gradient tensor associated with PSC is:

\[ \mathbf{L}^{\text{psc}} = \begin{bmatrix} \dot{\varepsilon} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\dot{\varepsilon} \end{bmatrix} \]  

(14)

Individual grains and grain boundaries, however, can evolve in a different way from the macroscopic applied deformation. Continuity in displacement and traction across all adjoining grain boundaries was enforced. The imposed strain rate was 0.001/s and the strain increments during numerical solution procedure ranged from 0.005 to 0.01. Regarding boundary conditions, the deformation was applied by imposing displacement to all nodes on the top in the negative 3-direction. Nodes in the bottom face, however, were constrained in the 3-direction (ND). Nodes on the front and back faces with normals in the negative 2- and positive 2-directions, respectively, were constrained in the 2-direction (TD). The right face with normal in the 1-direction (RD) was free while the left face was constrained in the -direction.

4. Results

4.1 Microstructure and texture changes after deformation and annealing

Figure 5 compares the deformation texture in the Zr and Nb phases after very large thickness reductions corresponding to a strain of 4.1. The characteristics of these textures have been analyzed in prior works. Generally it was reported that the rolling textures of the individual phases in the composites are consistent with the rolling textures of Zr and Nb when rolled alone
Using the initial texture as input, these deformation textures have been successfully predicted using both mean-field polycrystal plasticity models (Knezevic et al., 2014e) as well as the crystal plasticity finite element model used here (Ardeljan et al., 2014a).

Experimental analyses reveal that there is a slight texture change after annealing (Fig. 5) (Carpenter et al., 2014b). Figure 6 compares two texture fiber plots of the Zr phase in samples before and after annealing. As shown, the annealed texture has several components that differ from those in the deformed texture. There is a decrease of the \{1\overline{1}\overline{2}10\}\langle1\overline{1}\overline{2}0\rangle and \{0\overline{2}\overline{1}3\}\langle10\overline{1}0\rangle components and an increase in the \{5\overline{5}\overline{10}29\}\langle1\overline{1}\overline{2}0\rangle and \{0\overline{5}\overline{5}\overline{1}7\}\langle10\overline{1}0\rangle components.

In addition, the Zr phase undergoes significant changes in grain structure after annealing (Carpenter et al., 2014b). The effect of an annealing treatment reflects in the reduction of statistically stored dislocation density and decrease in orientation gradients in the microstructure. In addition, the grain size and shape have changed. Specifically, the grains have transformed from an elongated to an equiaxed shape and increased substantially in size (approximately 6 times).

For the fine layer thicknesses studied here, the changes in the microstructure of Nb after annealing were far less significant than those in Zr (Carpenter et al., 2014b). This difference is not surprising since the annealing temperature 575°C used is substantially lower than the melting temperature of Nb (2,477°C). In particular, changes in texture were minimal, a result that agrees with prior texture analyses performed on ARB Cu/Nb composites (Carpenter et al., 2014a; Carpenter et al., 2012).
Figure 5 Pole figures showing measured texture in Zr/Nb at 30 µm layer thickness (a) after deformation and (b) after annealing.

Figure 6 ⟨1 1 2 0⟩ and ⟨1 0 1 0⟩ fiber plots for 30 µm layer thickness Zr showing the effect of annealing on texture changes. Annealing leads to (1) a slight decrease of the overall ⟨1 1 2 0⟩ fiber fraction and a reduction in {1 1 2 10}(1120) component with an increase in {5 5 10 29}(1120) component and (2) a decrease of the overall ⟨1 0 1 0⟩ fiber fraction with a reduction in {0 2 2 13}(1010) component and an increase in {0 5 5 17}(1010) component.

4.2 Simulations of layered Zr/Nb in rolling

In a deforming two-phase polycrystal, the texture, grain size, grain shape, interface, and dislocation density can affect where and when strain (and strain rate) concentrations develop. The above experimental analysis indicates that many significant changes in texture and
microstructure occurred after intermediate annealing. Any of these or a combination of these factors could have contributed to the suppression of shear banding associated with application of intermediate annealing treatments. To provide some insight into how these changes affected the onset of this instability, we employ the modeling approach described in section 3 to: 1) examine the onset of strain localizations in the Zr/Nb composites (Section 4.2.2), 2) correlate them with microstructural features (Section 4.2.3), and 3) use this understanding to study the effects of annealing-induced microstructural changes on strain localizations in subsequent deformation (Section 4.3).

4.2.1 Boundary conditions at the Zr/Nb interface

As an important part of developing the model microstructure, we explored two options for representing the interface between the Zr and Nb phases using finite elements. In the first case we used a conformal mesh (one object representing both phases) and in the second case we used a non-conformal mesh with sticking boundary conditions between two objects (one object is the Zr phase and another is the Nb phase). Generating the former is more challenging since DREAM.3D is currently not capable of creating the two-phase lamellar microstructures that we need here. Therefore, we had to perform substantial manipulation of the voxelized microstructure data to ensure grain surface meshes between phases. To assess the effect on deformation behavior with these two options, we performed the plane strain simulation using one or the other. Figure 7 compares the equivalent plastic strain (PEEQ) contours after an ARB pass to a strain of 0.5 for the two cases. We find that the results are almost indistinguishable, and therefore, hereinafter use sticking boundary conditions at the Zr/Nb interface.
Figure 7 (a) Fully conformal FE mesh between grain boundaries and the two phases vs. (b) FE mesh with conforming elements between grain boundaries per individual phases and non-conforming elements between the two phases. The sticking boundary conditions are applied between the phases. Equivalent plastic strain contours after an ARB pass to a strain of 0.5 with (c) conformal mesh and (d) non-conformal with sticking between the layers. (e) Comparison of equivalent plastic strain at the interface planes for conformal and non-conformal meshes.
4.2.2 Strain localizations and formation of localized bands of strain concentrations in rolling

In this section, we analyze the evolution of strain fields within the developing microstructure under plane strain compression. Generally, when a polycrystal is subjected to mechanical deformation, an inhomogeneous strain field develops consisting of both areas of relatively high and low strain concentration. The areas of high strain are associated with large numbers of gliding dislocations, a response that can trigger shear banding. In the analysis that follows, we will refer to the outstandingly high strain concentration areas as hot spots and low concentration areas as cold spots and seek to understand which microstructural features are tied to hot and cold spot development.

To represent the initial texture, crystallographic orientations from a measurement of the initial texture were randomly picked and assigned to grains in the microstructure. In doing so, two issues arise. First, clearly, in carrying out this method, we would like to obtain the same initial texture if we were to randomly select another set of orientations from the same initial texture. Thus, it is important that the number of grains in the model is sufficiently large such that the texture and even the initial misorientation distribution are insensitive to the assignment of the grains. Second, in most of the simulations that follow, we will use the initial texture from the neutron diffraction measurement. However, as mentioned earlier, the initial texture for the same sample has also been measured by EBSD (Knezevic et al., 2014e). Thus, we repeated the plane strain compression simulations using different orientation assignments from either the neutron diffraction or EBSD texture in order to check if the general trends are dependent on how the initial texture was measured. Due to the slight differences in the measured texture some difference in the response is expected.
Figure 8 shows a 3D and 2D views of the strain concentrations and strain rate concentrations after deformation to a strain of 1.4 for all three cases of initial texture: two assignments from the EBSD texture (labeled EBSD 1 and EBSD 2) and one from the neutron diffraction texture (labeled NEUTRON). The imposed strain rate was 0.001/s. In all cases, the bulk textures calculated after the deformation simulation were nearly the same.

To identify the areas of high strain concentration, strains and strain rates that lie above 1.4 are colored in red. In all cases of initial texture, we see localized bands of high strain and strain rate concentration forming across the grain boundaries at approximately 35º from the rolling plane. Figure 8 also shows the interior of the samples, where more of these extended band-like strain concentration regions are seen. Whether they form appears to be independent of how the initial texture was assigned to the grains. Details on where they form, however, were the main distinction between the three cases, which merely indicates that grain and grain-neighbor properties matter.

We also should note that the areas of strain concentration are seen to be consistent with the areas of the strain rate concentration. Thus, hereinafter we analyze only strain concentration contours.
Figure 8 Distributions of equivalent strain (PEEQ) and equivalent strain rate (PEEQDOT) in the 3D model and in a 2D section at the strain level of 1.4. The strain level corresponds to the difference between two ARB passes i.e. from the 2.7/16/127 to the 4.1/64/30 (see Fig. 1).
4.2.3 Onset of hot spot formation

To determine how these band-like strain concentrations developed, we analyzed these same regions after true strains of 0.1 and 0.2, since by a 0.4 strain level, localized strains have already begun to develop between the hot spots creating a band-shaped configuration. Figure 9 shows the strain concentration distributions (normalized PEEQ with the applied strain) at these two strain levels for the case in which the initial texture was shown in Fig. 3b. As mentioned earlier, the initial texture in the other cases was similar and in using them, we found that band-like configurations of localized strain formed were also similar. The following findings were common to all three.

We first note that more often, the more intense localized hot spots begin in the Zr phase, not the Nb phase. This observation suggests that hot spot initiation is related to areas where strain accommodation is difficult. Low symmetry HCP crystals have less available slip modes (less degrees of freedom) for accommodating deformation than cubic crystals. Zr is highly anisotropic and in large strain deformation deforms predominantly via three modes of slip {a} prismatic, {c + a} pyramidal, and {a} basal, possessing different hardening characteristics (Knezevic et al., 2013b). Nb is also plastically anisotropic but has many more slip systems, among say the two modes of slip, {110}{111} and {112}{111} slip, and exhibits a lower hardening rate than an HCP metal.

Second, it is found that hot spot strain concentrations develop primarily at particular triple or quadruple junctions, where three and four grains meet in a 2D section and not in interior of the grains. Again, this result suggests that hot spot generation starts in areas where local strain accommodation is challenging. Grain junctions are regions where accommodating grain
deformation among distinct grains while maintaining compatibility (i.e., no cracking) could be problematic if the bulk distortions between neighboring grains are disparate.

Last, under further straining (0.2 strain level), these special regions of strain concentration extended from the triple junctions, non-preferentially into all the adjoining grains. This observation implies a weak or insignificant influence of individual grain properties. Beyond 0.2 strain level, these hot spots link to form a band-shaped strain concentrated region. This indicates that hot spots formation would eventually drive concentrated band formation.

A 3D grain structure contains many regions where three or more grains meet but as seen in the above simulations, the hot spots in strain concentrations develop in only a small percentage of them. In fact, most triple junctions or quadruple points (in a 2D section) do not form a hot spot and do not participate in eventual formation of a strain concentration band. In fact, the same grain can be connected to multiple junctions and after some amount of deformation, all or most of these junctions will not develop a hot spot.

**Figure 9** Distributions of normalized value of equivalent plastic strain (\(\overline{\text{PEEQ}}\)) at true strains of 0.1 and 0.2 showing strain heterogeneities developing at grain boundaries and triple/quadruple junctions. Red circles indicate hot spots forming a band. Black circles indicate hot spots disappearing and not forming a band. Blue circles indicate cold spots.
To understand the special properties of hot spots, we examined a large number of hot spots and cold spots at 0.1 and 0.2 strain levels. Based on our threshold values, cold spots have a very low strain concentration (less than 0.5) and show as ‘blue’ and the hot spots have a relatively large strain concentration (greater than 1.2) and show as ‘red’ in the contour maps. Interestingly, like hot spots, cold spots corresponded to regions where three or more grains meet and had a strain concentration that is even lower than the strains within the interiors of grains. A similar outcome was reported previously in a study of deformed FCC polycrystals, using another 3D full-field crystal plasticity model based on a Green’s function homogenization scheme (Rollett et al., 2010). There it was also seen that both hot and cold spots in stress were generated at grain boundaries, triple junctions, and quadruple points.

Since it appeared that hot spots corresponded to areas where maintaining compatibility across neighboring grains was difficult, we compared the deformation properties (shear strain, average strain, lattice reorientation) of the three or four grains associated with each hot and cold spot. In doing this, we selected a center of the hot/cold spot to be the peak strain level and constructed a sphere around it. Our key finding is that differences in reorientation tendency were the most distinguishing characteristics between cold and hot spots. Figure 10 shows the variation in misorientation of each grain belonging to a spot from its original orientation after 0.1 and 0.2 strains. Comparing the left plot for hot spots with the right one for cold spots, we find that hot spots are grain junctions that join grains with significantly disparate reorientation propensities during deformation, and vice versa, cold spots join grains that have similar reorientation propensities. Results in Fig. 10 for 0.2 show that the dispersion among the grains joined at a junction appears to grow as straining continues. From these results, we can conclude that areas of high strain concentration initiate at points where many grains with significantly different
reorientation tendencies meet. Figure 11 shows the formation of banded configurations crossing many grains from hot spots that are close in proximity and well aligned along the macroscopic direction of shearing.

**Figure 10** Crystallographic reorientation of grain sets selected to belong to (a) hot and (b) cold spots for three realizations of the microstructure at strain levels of 0.1 (top row) and 0.2 (bottom row).
Figure 11 Distributions of normalized value of equivalent plastic strain ($\bar{\varepsilon}_{PEEQ}$) at a true strain of 0.4 showing a trans-granular localized band.

4.3 Effect of the microstructural changes after annealing on strain localization

In this section, we systematically study the role of annealing-induced microstructural changes on strain localization during subsequent rolling. We focus on the Zr phase because significantly more of the hot spots originate in the Zr. To this end, we started with the deformed microstructure after a strain level of 1.4 (Fig. 8) and then subsequently altered the Zr microstructure to reflect the main consequences of annealing that were observed experimentally. We identified the following cases, each reflecting particular changes in the microstructure due to annealing: (case 1) the dislocation density reduced to a small value of $10^{12}$ m$^{-2}$, while maintaining the deformed structure and orientation gradients; (case 2) the dislocation density reduced to $10^{12}$ m$^{-2}$, the orientation gradients removed, and the annealed texture (Fig. 5b) assigned to the deformed grain structure; and (case 3) the grain structure changed to correspond to the equiaxed recrystallized grains, the dislocation density reduced and annealed texture assigned. While case 3 best represents the Zr microstructure after annealing, cases 1 and 2 are intended to isolate individual effects. While residual stresses can also play a role in the localizations, it is assumed that annealing has minimized their effects in all cases studied here.

Figure 12 shows the 3D microstructure models for each case. The grains are colored by the inclination angle $\theta$ from the ND of the c-axis for the Zr grains and the [001] axis for the Nb.
grains. In case 1, the grain shape is elongated in both Zr and Nb due to the prior rolling to a strain level of 1.4. The deformation textures are those typical of rolled Zr and Nb (Ardeljan et al., 2014a; Ardeljan et al., 2014b) where grains have achieved preferred orientations. Because the dislocation density has been reduced to $10^{12} \text{ m}^{-2}$ in this case 1, any intra-granular and inter-granular gradients in dislocation density caused by the prior straining have been removed. However, as shown, the intra-grain orientation gradients during prior rolling remain. In case 2, we have additionally re-assigned the texture to that after the intermediate annealing treatment. Specifically, the orientations are sampled at random from the measured annealed texture (Fig. 5b) and reassigned at random to the grains in Fig. 12. The texture difference in the case 2 model microstructure can be readily seen by the difference in grain color maps of $\theta$. An additional consequence is that the orientation gradients caused by the prior 1.4 plane strain deformation also have been removed. It should be noted again that cases 1 and 2 are hypothetical cases since grains after anneals that remove stored dislocation density and orientation gradients usually do not retain the elongated grain shape typical of heavy rolling. That said, we present case 3, which, as shown, is distinct from cases 1 and 2 in that the grain structure for Zr is created to represent the changes due to annealing. The grains have increased by six times and have become nearly equiaxed. As in cases 1 and 2 the stored dislocation density has been reduced and the grain orientations have been assigned the annealed texture in Fig. 5a. The microstructures corresponding to the three cases were then deformed in plane strain compression for an additional strain of 0.4 and their tendencies to develop hot spots and eventual large bands of strain concentration were evaluated. To facilitate fair comparisons and improve the accuracy of these simulations, a new FE mesh of approximately the same number of elements as in the original FE model (Fig. 4b) has been used in all simulations from 4.1 to 4.5 total strain.
Figure 12 Microstructure models of the 30 µm layered composite representing changes after annealing. Individual grains are identified based on the inclination angle $\theta$ of the crystallographic c-axis for HCP and [001] for BCC relative to the sample ND. Corresponding FE models for subsequent deformation consisted of approximately 1.5 million C3D4 (continuum 3D 4-node) tetrahedral elements.

In order to confidently discuss that hindrance of bands after a stain of 4.1 is due to the intermediate annealing, Fig. 13 shows results of the simulation of non-annealed microstructure. Note that the states of microstructure and residual stresses have not been altered as they will be after annealing. The plots clearly show that localizations increase with continuous straining.

Figure 13 Distribution of equivalent strain normalized by the applied equivalent plastic strain after subsequent straining of non-annealed microstructure (Fig. 8) from 4.1 to 4.5 total strain.
**Case 1:** Figure 14 shows the normalized equivalent plastic strain using the applied strain contours after an additional strain of 0.4. The full length of the strained sample is presented for three sections in the (RD, ND) plane (at 10% from the front face, the center plane, and at 25% from the back face). Like the material deformed to the same 0.4 strain after a few rolling passes (Fig. 11), we see the localizations start in Zr and occur at grain boundaries. However, in many ways this case exhibits a different response. The strain localizations are smaller in magnitude and more sparsely distributed. They do not have a tendency to link and form the expected 35-40° inclination bands in any of the sections, but instead cross several grains following the grain elongated grain shape. To see more clearly how they correlate with the microstructure, we zoom-in on the central regions (for example) where the details of the grain structure can be examined. Increased aspect ratio of grains causes the strain bands to preferably propagate horizontally. These results for *case 1* show that the reduction in stored dislocations caused by annealing helps postpone the formation of inclined bands of strain localization.

**Figure 14** Distribution of equivalent strain normalized by the applied equivalent plastic strain after subsequent straining of the *case 1* (see Fig. 12) microstructure to a strain of 0.4.
Case 2: For the case 2 microstructure, we repeated the simulation of plane strain compression to a 0.4 strain level. As in the deformed case and post-annealed case 1, the localizations start in Zr and occur at grain boundaries. As in case 1, there is no obvious propensity to form localized transgranular strain bands at 35-40° from RD in any of the sections. Instead, areas of local strain concentration are dispersed occasionally within the Zr phase. However, from the resulting normalized strain contours shown in Fig. 15, we find that the number of concentrated strain regions is slightly increased compared to case 1 for the same sections and after the same amount of strain. Evidently, although reductions in stored dislocation density had a profound effect, we see here that removal of orientation gradients and re-initialization of the deformed texture to the annealed texture led to a slight increase of localized strained regions due to the introduction of crystallographic incompatibilities between previously stabilized grains. It should be noted that among the annealing cases, the state of the microstructure and residual stress in case 2 is the most similar to the initial state of the microstructure for the 2.7 to 4.1 deformation. The inhibition of the shear band formation in case 2 can be associated to a combination of elongated grain shapes and annealed texture.

Figure 15 Distribution of equivalent strain normalized by the applied equivalent plastic strain after subsequent straining of the case 2 (see Fig. 12) microstructure to a strain of 0.4.
**Case 3:** Case 3 best represents the actual microstructure after annealing. It should be noted that surface effects due to the uniform-displacement boundary conditions applied on the top and bottom surfaces can lead to a stiffer material response. For this reason we have performed simulations with a grain size that is two times smaller (not experimentally informed). We observed a similar response. Our discussion below is based on the interior grains of both simulations. For the starting case 3 microstructure, Fig. 16 plots the corresponding strain concentration contours after 0.4 strain. Similar to the deformed structure and post-annealed cases, areas of higher strain concentration are found firstly in Zr and predominantly at grain boundaries and junctions. Like cases 1 and 2, the sequence of hot spot generation and subsequent connection does not occur. In contrast, although the texture is the same as in case 2, we see that a higher volume of high strain concentration appears in case 3 than case 2. These large ‘hotter’ areas follow the grain shape and correspond to the plastically softer grains that are accommodating more of the applied strain. These softer grains also develop a more homogeneous strain field across their volume.

To summarize, the common feature of all four situations (as deformed Fig. 11, and post-anneal cases 1, 2, and 3) is that localized hot spots in strain start in Zr and occur at grain boundaries and junctions. Bands have not developed in any of the annealed cases indicating that the reduction in dislocation density was the dominant factor. While it may be difficult to avoid strain localizations at grain junctions, when provided a microstructure containing a large few grains spanning the thickness, elongated grain shapes, and reduced dislocation density, the linkage of hot spots in the form of a band can be postponed.
4.4 Demonstration of strain localization leading to shear banding

The strain concentrations studied here can lead to shear banding. The foregoing calculations find that they most often develop first in the Zr phase. This observation suggests strongly that shear bands are more likely to initiate in the Zr phase than at the Zr/Nb interface or within the Nb phase. For demonstration, we carry out a final simulation in which areas of high strain concentration are plastically softened, that is, if the strain concentration exceeds 1.0, the area is given a value of dislocation density corresponding to the annealed condition $10^{12}$ m$^{-2}$. Figure 17 shows the starting state of the microstructure when softening has been introduced. Figure 18 shows the normalized strain contours after a strain of 0.2 after this softening mechanism has been incorporated. As shown, the subsequent deformation leads to the formation of a shear band and within these bands, the strain is on average six times that of the material immediately outside of these bands.

This last simulation was intended for proof of principle only since our interests in the present work lie in the microstructure-driven events leading up to strain localizations and not the
modeling of shear banding, which would follow strain localizations. For a more physical description of the transition from strain concentrations to shear band formation, it would be desirable to incorporate a model for localized heating due to the rapid glide of groups of dislocations associated with the highly strained areas. The heating in effect reduces the resistance to glide, causing a local reduction in the flow stress.

Figure 17 2D section at TD=0.1 of the deformed 3D model (Fig. 8) at the strain level of 1.0 used for the subsequent straining with softening induced in the localized areas: (a) distributions of equivalent strain and (b) mesh of the current grain structure.

Figure 18 Shear banding after softening elements experiencing hot spots: (a) deformed grain structure and (b) distributions of equivalent strain normalized by the applied equivalent plastic strain after subsequent straining of 0.2.

5. Conclusions

In this work we present a 3D microstructure based, multi-scale crystal plasticity finite element (CPFE) model. We apply it to understand the relationship between microstructure and
strain localizations during plane strain compression of a two-phase hexagonal closed-packed/body-centered cubic (HCP/BCC) Zr/Nb lamellar composite. Experimentally informed representations of the deformed or annealed polycrystalline grain structures within Zr/Nb micron-layered composites were constructed in DREAM.3D. A meshing toolset was then developed to mesh the grains and grain boundary network within these DREAM.3D microstructure models. The constitutive model used a dislocation density based hardening law, wherein the dislocation densities for the multiple modes of slip in Zr and Nb evolve with their own individual dependencies on strain, temperature, and strain rate. With this multi-scale modeling approach and DREAM.3D microstructural representations of grain topology, we have helped to better link microstructure with the strain localizations that can precede the development of shear bands. The studies provide insight into the relationship between grain structure and the onset of strain localization. The main conclusions of this work are as follows:

- Localized spots of strain concentrations (hot spots) initiate in the Zr phase as opposed to the Nb phase. This finding helps to explain why intermediate annealing, which greatly affected the microstructure of the Zr, had a significant impact on the development of strain instabilities.

- Hot spots form at grain junctions that join at least three or four grains with significantly disparate reorientation propensities during deformation. Vice versa, cold spots form at junctions where the adjoining grains have similar reorientation propensities.

- As straining continues, these hot spots in strain concentration link to create localized bands that cross many grains from one Zr/Nb interface to the next.

- The microstructure of the Zr phase was altered to represent the effects of post-annealing treatments. In spite of reductions in dislocation density, changes in texture, and increased
grain size, strain localizations (hot spots) still initiated at grain junctions in the Zr phase after straining. The results suggest that when a layered microstructure has a few large grains spanning the layer thickness, elongated grain shapes, and reduced dislocation density, the linkage of hot spots in the form of a band can be postponed.

Acknowledgements

MK and MA acknowledge subcontract, NO. 277871, granted by Los Alamos National Laboratory to the University of New Hampshire. IJB, TMP, and NAM wish to acknowledge support by the UC Lab Fees Research Program # UCD-12-0045.15. TN was supported by the Department of Defense (DoD) through the National Defense Science & Engineering Graduate Fellowship (NDSEG) Program.

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Zr/Nb nanolayered composites processed by accumulative roll bonding. IOP Conference Series: Materials Science and Engineering 63, 012170.


Chapter 4

This chapter was published as: The plasticity of highly oriented nano-layered Zr/Nb composites, Milan Ardeljan, Daniel J. Savage, Anil Kumar, Irene J. Beyerlein, Marko Knezevic, Acta Materialia, 115, 189-203. My role in preparing this chapter was to perform a parametric study in order to investigate and to better understand the orientation stability of nanocrystalline Zr during accumulative roll bonding process. This involved modeling of Zr/Nb bicrystals during rolling and post-processing of the data presented in this chapter. Furthermore, I contributed by writing several sections in the paper that mainly addressed the modeling aspects of the performed work, as well as designing and preparing most of the presented figures and graphs.
The plasticity of highly oriented nano-layered Zr/Nb composites

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Abstract

In prior work, bulk lamellar composites of pure zirconium and niobium (Zr/Nb) were manufactured by accumulative roll bonding (ARB). After the substantial amounts of straining required to refine the layers to nanoscale dimensions, formation of highly oriented Zr crystals was observed. In this work, we employ a spatially resolved multiscale crystal plasticity based model in 3D to study the orientational stability of Zr single crystals and Zr/Nb bicrystals during rolling deformation. The analysis reveals that predominant texture components arise due to substantially reduced ratios of slip resistances among the prismatic, pyramidal I \(\{c + a\}\), and basal slip systems. In support, density functional theory (DFT) calculations of generalized stacking fault energy curves on these three slip systems suggest that the ratio of critical stresses to form these dislocations are within 2.5 times. This finding of reduced anisotropy in Zr at the nanoscale can provide insight into the design of nano-structuring processes for target textures, such as those containing highly oriented grains.

Keywords: Zirconium; Niobium; Crystal plasticity; Accumulative roll bonding; Interfaces

1. Introduction

When subject to bulk metal forming processes, such as rolling, polycrystalline metals develop texture [1, 2]. Texture affects both mechanical [3-5] and functional properties [6, 7]. As such, control of texture evolution during processing is an approach often used to help attain
target properties and eventual performance [8-12]. For hexagonal close packed (HCP) metals, such as Zr, Mg, Ti, and Be, a preferred texture develops after some amount of straining, and if its components are orientationally stable, is maintained with further straining [13-18]. Under the severe plastic deformation process, such as accumulative roll bonding (ARB) [19], it has been shown that the characteristic rolling texture of Zr persists even up to large strains of 10 [20, 21].

Recently ARB has been applied to a two-phase Zr/Nb composite with the aim of using the biphase interfaces to help refine the Zr phase to nanoscale dimensions [22]. Figure 1 shows micron- and nano-layered Zr/Nb composites made by ARB. Starting with $h = 1$ mm layer thickness, ARB was successfully used to reduce the layer thickness from hundreds of microns (Fig. 1a) to less than 100 nm (~92 nm) as seen in Fig. 1b, while keeping a continuous layered architecture, hence achieving a nanolayered Zr/Nb composite. There have been other attempts to achieve <100 nm microstructures of Zr, but these resulted in non-uniform distributions of nano to submicron grains or phase transformations [23-28].

**Figure 1** Lamellar microstructures in the Zr/Nb composite produced by the ARB process: (a) optical micrograph showing the structure when the average layer thicknesses approximately 106 µm at a strain level of approximately 2.9 and (b) transmission electron microscopy diffraction contrast image showing the structure when the average layer thickness is approximately 92 nm at a strain level of approximately 10.
The Zr phase maintained a conventional rolling texture characteristic of single-phase Zr until \( h \) was refined below 100 nm, at which point the texture consisted of even fewer components. For instance, orientations with their crystallographic c-axis aligned with the normal direction (ND) of the sheet are contained within the texture of rolled coarse-grained Zr, but they disappear when the Zr layers are refined below 100 nm.

Loss of orientational stability suggests that slip activity within the grains has changed, despite the fact that the same rolling deformation state is applied. When the layer thickness is reduced below 100 nm, the nano-layered structure, the layers are spanned by only one crystal and thus every Zr grain is bonded to a Nb grain. First, a change in slip activity could arise at the nanoscale because the Zr crystals must deform while at the same time meeting compatibility constraints with neighboring Nb crystals. There may be some Nb orientations for which meeting the compatibility criterion is easier than others. Second, in nanoscale grains, dislocations no longer primarily originate from the grain boundaries or the interior of the grains, but at the phase interfaces. The phase interfaces serve as nucleation sites, annihilation sites, and barriers. It is, therefore, possible that the change in slip activity occurs because the critical stresses for activating dislocations are determined by the nucleation barrier from the interfaces, not the internal crystal defects and grain boundaries. It is also likely that the critical stress to activate dislocation motion (or critical resolved shear stress, CRSS) is dominated by the nano-scale mean free path between adjacent interfaces and again, not by the dislocations that are stored within the layers. Last, the stresses that develop during rolling of such fine nanograins are much higher than those achieved in a coarse-grained polycrystalline Zr and therefore could even enable the more difficult slip modes (such as basal slip) to activate.
The aim of this work is to understand the orientation stability of nanocrystalline Zr during ARB. We use a crystal plasticity based model that allows for slip to occur on available slip modes and can directly relate texture evolution to the relative contributions of different slip modes. The analysis indicates that Zr crystals, when bonded to Nb crystals, become less orientationally stable than the same single crystal orientation under the same deformation state. We show that the “nano-preferred” texture components arise when the plastic anisotropy of Zr is substantially reduced, in which the slip resistance ratio of prismatic slip to basal slip or to pyramidal slip have decreased below 2.0. In support of this finding, we perform density functional theory (DFT) calculations of generalized stacking fault energy curves on these three slip systems and they indicate that the stresses to form these dislocations are indeed close (within 2.5 times). Although we focus this study on nanocrystalline Zr, the findings are sufficiently general to provide insight into mechanisms underlying the nanotruturing SPD processes of other HCP metals that can be refined to nano grained structures.

2. Background

2.1 Stable orientations in coarse-grained Zr

The materials used in this study are high-purity Zr with the following chemistry expressed in weight parts per million (Wt. ppm) Hf = 35, Fe < 50, Al < 20, V < 50, O < 50, N < 20, C < 22 and Zr balance [29] and reactor-grade high-purity Nb (99.97% pure, ATI-Wah Chang). As we mentioned in the introduction, recently ARB was applied to 50/50 Zr/Nb, involving high-purity Zr and Nb [22, 27]. The process refined the layer thicknesses \( h \) from 1 mm to 92 nm. Figures 2 and 3 show pole figures and the \( \langle 11\bar{2}0 \rangle \) and \( \langle 10\bar{1}0 \rangle \) fibers for the Zr phase, respectively, for three layer thicknesses. From layer thicknesses \( h = 1 \text{ mm} \) down to \( h = 26 \mu\text{m} \), the texture that developed in the Zr phase was very close to the conventional one and the \( h = 106 \mu\text{m} \) Zr/Nb
composite shown in Fig. 1a, is one example. For these layer thicknesses, the layers were polycrystalline, with 10 to 20 grains spanning the thickness of the layer. The basal pole figure of the Zr phase exhibits a split peak in the TD, a characteristic feature in the texture of Zr when rolled alone. The peaks are not pronounced with intensities ranging from 4-6 multiples of random distribution (mrd) over a range of basal pole tilt from 0° to 30° from the ND.

We identify seven Zr orientations in the rolled texture of coarse-grained Zr. Usually among these preferred ones, none of them are strongly favored over the other. Along the \(\langle 11\bar{2}0 \rangle\) fiber for \(h = 106\ \mu\text{m}\), there are three chief Zr orientations, starting with the basal pole component aligned with the ND (Zr1) and spanning 30° from the ND (Zr2 and Zr3). Along the \(\langle 10\bar{1}0 \rangle\) fiber, there are four main orientations, including the basal pole component along the ND (Zr4) and covering orientations tilted up to 45° from the ND (Zr5-Zr7). These orientations are mapped onto a basal pole figure in Fig. 4 and listed in Table 1.
**Figure 2** Pole figures showing the deformation texture in the Zr phase of the rolled Zr/Nb composite to (a) 106μm, (b) 92 nm and (c) 41 nm layer thickness.
Figure 3 (1 1 2 0) and (1 0 1 0) fiber plots for the Zr phase in the Zr/Nb ARB composites with nominal 106 μm, 92 nm and 41 nm Zr layer thickness.

2.2 Anisotropy of Zr

In an attempt to determine the slip modes that contribute to the stable rolling texture of the Zr phase during manufacturing of the Zr/Nb composite, two types of crystal plasticity models were employed, both utilizing the same Zr hardening law [30]. The earlier attempt involved a mean-field technique and modeled Zr and Nb as separate phases, and the latter one, used a full-field model, and simulated the deformation as two phases co-deforming (compatibility across the dissimilar phases). Both models were successful at modeling texture evolution in the Zr phase in the coarse-layered Zr/Nb composite, in which the calculated texture had the basal poles spread from the ND to the TD with some weak peaks forming off ND, ranging from 10° to 35° from the ND. This calculated texture was similar to that texture of single phase Zr rolled alone [20, 31]. Both models also used the same hardening law for Zr and the set of critical resolved shear stresses (CRSS) for prismatic (a) slip, pyramidal I (c + a) slip and basal (a) slip. Under the
conditions of rolling modeled here (room temperature, moderate strain rate deformation), the initial CRSS values for prismatic \( \langle a \rangle \) slip, pyramidal \( \langle c + a \rangle \) slip and basal \( \langle a \rangle \) slip were 12 MPa, 133 MPa, and 142 MPa, respectively [32].

Both Zr/Nb plasticity models found that while all three slip modes were active during rolling, they were not equally contributing. Prismatic \( \langle a \rangle \) slip dominated in accommodating the rolling strain, with pyramidal \( \langle c + a \rangle \) slip contributing secondly, and basal \( \langle a \rangle \) slip, contributing a minor amount. The result is consistent with the prior peak broadening measurement on a Zr alloy [33]. Thus, it was shown that the conventional rolling texture and the Zr phase texture in the coarse-layered composites were a result of the significant plastic anisotropy of Zr, with prismatic slip being predominant.

2.3 Stable components in nanoscale Zr

An interesting transformation in texture development arises when nanolayered thicknesses in the Zr/Nb composites \( (h = 92 \text{ nm}) \) are achieved [22]. The Zr phase texture becomes highly oriented and deviates from the conventional rolled Zr texture. To demonstrate, the fiber plots in Fig. 3 include the textures for the \( h = 92 \text{ nm} \) and \( 41 \text{ nm} \) Zr/Nb ARB composite. As shown, compared to the micron-layered composite, in the 92 nm composite, the basal components, Zr1 and Zr4, have decreased in intensity and those of Zr2, Zr3, Zr5, Zr6, and Zr7, have increased. As the layers were refined to \( 41 \text{ nm} \) the basal components Zr1 and Zr4 continue to drop, while Zr2-3 and Zr6-7 continue to strengthen. This nano-scale induced transformation signifies a change in orientation stability. Orientational stability can be altered by a change in slip activity, a general term that refers to the number of active slip systems, the mode(s) involved, and the distribution of slip across the activated slip systems.
Figure 4 Basal pole figures showing location of the seven Zr components whose stability under rolling is studied in this work.

There are two possible ways worth pursuing in which slip activity in nanocrystalline Zr could have been altered. The first concerns the increased compatibility constraint arising in the nanolayered composite. When the layers refine to the nanoscale, only one crystal spans the layers, so every Zr grain becomes bonded to a Nb grain. Satisfying compatibility so that the Zr/Nb co-deform could have altered slip activity in the Zr. The second possibility is an alteration in the activation stresses for the three available slip systems, prismatic, basal, and pyramidal. Although other ways are possible, it is clear that these two prospects warrant investigation.

<table>
<thead>
<tr>
<th>#</th>
<th>Zr ( (\varphi_1, \phi, \varphi_2) )</th>
<th>Nb ( (\varphi_1, \phi, \varphi_2) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( (0^\circ, 0^\circ, 30^\circ) )</td>
<td>( (0^\circ, 0^\circ, 45^\circ) )</td>
</tr>
<tr>
<td>2</td>
<td>( (0^\circ, 17.5^\circ, 30^\circ) )</td>
<td>( (0^\circ, 25.24^\circ, 45^\circ) )</td>
</tr>
<tr>
<td>3</td>
<td>( (0^\circ, 25^\circ, 30^\circ) )</td>
<td>( (0^\circ, 35.26^\circ, 45^\circ) )</td>
</tr>
<tr>
<td>4</td>
<td>( (0^\circ, 0^\circ, 0^\circ) )</td>
<td>( (0^\circ, 46.69^\circ, 45^\circ) )</td>
</tr>
<tr>
<td>5</td>
<td>( (0^\circ, 15^\circ, 0^\circ) )</td>
<td>( (0^\circ, 54.74^\circ, 45^\circ) )</td>
</tr>
<tr>
<td>6</td>
<td>( (0^\circ, 25^\circ, 0^\circ) )</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>( (0^\circ, 45^\circ, 0^\circ) )</td>
<td></td>
</tr>
</tbody>
</table>

Table 1. Selected Zr and Nb orientations studied here for their orientational stability in rolling.
The goal of this work is to employ a multiscale model built upon a crystal plasticity finite element (CPFE) framework to examine these two ways in which slip could have been augmented within nanocrystalline Zr phase to drastically change its orientational stability in rolling. We first briefly review the CPFE model. In what follows, we first apply the model to investigate the orientational stability of single crystal Zr using the activation barriers for slip characteristic of coarse-grained Zr. To investigate the effects of co-deformation with Nb on the orientational stability of coarse-grained Zr crystals, we study the deformation of bicrystals of Zr/Nb. To determine whether there has been a change in activation barriers for slip, we then repeat the single crystal Zr and bicrystal Zr/Nb analysis with the resistance values for the three available slip systems, prismatic, basal, and pyramidal, altered for nanocrystalline Zr.

3. Modeling

3.1 Summary of the CPFE constitutive law

In CPFE, the deformation of every material integration point in the mesh in Fig. 9 follows a constitutive law based on elastic anisotropy and rate-dependent crystallographic slip. We summarize briefly the formulation and refer the reader to [34-38] for more details.

In the finite deformation formulation, the total deformation gradient tensor $F$ is decomposed into an elastic $F^e$ and plastic $F^p$ parts via:

$$F = F^e F^p,$$

(1)

where $F^e$ is comprised of deformation gradients from elastic stretching and lattice rotation. The relationship between $F^e$ and stress is given by:

$$T^e = CE^e, \quad T^e = F^{-1} \{ (detF^e)\sigma \} F^{-T}, \quad E^e = \frac{1}{2} \{ F^{eT} F^e - I \},$$

(2)

where $T^e$ and $E^e$ are work conjugate stress and strain measures, $\sigma$ is the Cauchy stress, and $C$ is the fourth-order elasticity tensor.
The evolution of $\mathbf{F}^P$ is governed by crystallographic slip according to:

$$\dot{\mathbf{F}}^P = \mathbf{L}^P \mathbf{F}^P, \mathbf{L}^P = \sum_s \dot{\gamma}^s \mathbf{b}_0^s \otimes \mathbf{n}_0^s, \mathbf{F}^P(\tau) = \{\mathbf{I} + \Delta \tau \mathbf{L}^P(\tau)\}\mathbf{F}^P(t),$$

where $\dot{\gamma}^s$ is the slip rate on slip system $s$, $\mathbf{L}^P$ is the plastic velocity gradient, $\mathbf{I}$ is the identity matrix, and $\mathbf{b}_0^s$ and $\mathbf{n}_0^s$ are the slip direction and the slip plane normal of $s$, respectively, in the undeformed configuration denoted by 0. The $\dot{\gamma}^s$ is related to the resolved shear stress ($\tau^s = \mathbf{T}^e \cdot \frac{1}{2} (\mathbf{b}_0^s \otimes \mathbf{n}_0^s + \mathbf{n}_0^s \otimes \mathbf{b}_0^s)$) and a characteristic shear stress ($\tau_c^s$) for slip system $s$, according to a power-law relationship [39-41]:

$$\dot{\gamma}^s = \dot{\gamma}_0 \left(\frac{\tau^s}{\tau_c^s}\right)^m \text{sign}(\tau^s),$$

where $\dot{\gamma}_0$ is a reference slip rate (taken here as 0.001 s$^{-1}$). The exponent $m$ is the strain rate sensitivity. Here it is set to 0.01, a value which applies to most metals at low homologous temperatures.

From $\mathbf{L}^P$ we can calculate the lattice spin $\mathbf{W}^e$ via

$$\mathbf{W}^e = \mathbf{W}^{app} - \mathbf{W}^P, \mathbf{W}^P = \frac{1}{2} (\mathbf{L}^P - \mathbf{L}^P^T),$$

where $\mathbf{W}^{app}$ is the spin applied to the polycrystal and $\mathbf{W}^P$ is the plastic spin. As shown in the right hand side of Eq. (5), $\mathbf{W}^P$ is the skew-symmetric component of $\mathbf{L}^P$. The integration of this constitutive model is performed using an iterative Newton-Raphson scheme [34].

3.2 Hardening law

For the evolution of the characteristic shear stress $\tau_c^s$ in Eq. (4) we use a dislocation density (DD) based hardening law formulation. The overall model is referred to be the DD-CPFE model. The model assumes that dislocations are stored according to thermally activated rate laws and as a consequence, the resistance stresses $\tau_c^s$ are a function of strain, temperature, and strain rate [30, 42-50]. This law is applied to every slip system $s$ in Zr and Nb. For Zr, we make available
prismatic \{1100\}\{\overline{1}20\} slip, pyramidal I \{10\overline{1}1\}\{\overline{1}23\} slip and basal \{0001\}\{\overline{1}20\} slip [30, 51-53]. Basal slip is the hardest slip system and known to occur only at larger strains, after the easier slip systems have strain hardened [26, 54-56].

For Nb, the \{110\}\{\overline{1}1\} and \{112\}\{\overline{1}1\} slip modes are made available for deformation. While we are aware that non-Schmid effects in BCC have been found to be important at certain conditions for capturing the plastic anisotropy [57-59], we neglect them in the calculations to follow. In both metals, deformation twinning is possible, but it tends to be profuse at temperatures lower than the room temperature conditions being modeled here or under a high strain rate deformation [60-62]. Moreover, twinning was not found prevalent in prior studies of ARB Cu-Nb and Zr-Nb nanocomposites [27, 54, 63]. The selected crystal orientations studied here are much more favorably oriented for slip than for twinning with respect to the loading direction. Therefore, twinning was not considered in this work.

4. Orientational stability of single crystal Zr

The model is first applied to study the orientational stability of single crystal Zr. Orientational stability depends on the initial orientation. Upon application of load, the crystal deforms elastically until the onset of slip on a combination of slip systems. Generally, the slip activity, being the number of active slip systems and distribution of shear among them, will contribute to the reorientation of the crystal from its initial orientation. As defined in Eq. (5), the total spin rate depends on the plastic spin rate and the spin rate contributed by the applied loading. The relationship between the plastic spin rate and the active slip systems is given by:

\[
\mathbf{W}^p = \sum \dot{\gamma}^s \frac{1}{2} (\mathbf{b}_0^s \otimes \mathbf{n}_0^s - \mathbf{n}_0^s \otimes \mathbf{b}_0^s).
\]

One indication of orientational stability would be negligible or zero total spin rate. The null result would imply that under that loading state, the slip activity that develops in this crystal
orientation is such that the initial orientation is maintained under loading. Positive spin rates signify orientational instability.

Here, we will study the orientational stability of Zr crystals in PSC, an approximation of rolling deformation. In PSC, the applied spin rate is zero, and thus, it is only necessary to analyze the plastic spin rate, which is a direct consequence of the slip activity. The plastic rate spin tensor $W^p$ can be represented by a scalar rotation rate angle,

$$\dot{\theta} = \sqrt{(W^p_{12})^2 + (W^p_{23})^2 + (W^p_{13})^2},$$

which is also called the pure spin rotating about an axis $n$ i.e., $W^p = N\dot{\theta}$, where $n$ is the dual vector of the unit anti-symmetric tensor $N$.

To relate orientational stability, we calculate the reorientation rate, $\dot{\theta}$ for single crystals with a given initial orientation under PSC. The 3D $\dot{\theta}$ contour maps were calculated over the entire orientation space, taking into account the HCP crystal symmetries. These symmetry operators can be found in the appendix A. The resulting orientation space is known as the HCP fundamental zone ($FZ$) $FZ = \{ g = (\phi_1, \Phi, \phi_2) \mid 0 \leq \phi_1 \leq 2\pi, 0 \leq \Phi \leq \frac{\pi}{2}, 0 \leq \phi_2 \leq \frac{\pi}{3} \}$ [64-67].

Figure 5a shows the $\dot{\theta}$ calculated at a total strain of 0.02. Here in the interest of space we only display the most relevant 2D sections of this $FZ$ on which the seven Zr orientations lie (see Table 1). In Fig. 5a, it can be seen that for most of the orientation space, Zr single crystals are not orientationally stable. The spin-rate analysis indicates that two of the seven key Zr orientations have negligible spin rates: Zr1 and Zr4. The other orientations, Zr2, Zr3, Zr5, Zr6, and Zr7 have positive spin rates, meaning that they are not as stable and would reorient away from these starting orientations. The results are consistent with the texture development in single-phase, coarse-grained Zr. In the texture that stabilizes in large-strain, room-temperature
rolling of Zr, the basal poles are distributed from the ND to the TD, indicating that none of these seven components are particularly preferred over the others [54].

For more insight, Figs. 5b-d present the \( \dot{\theta} \) resulting from the individual slip modes. From the analysis we find that the instability of orientations in PSC arises from the prevalence of prismatic slip. Basal slip would not lead to a significant reorientation but pyramidal slip could render some of the orientations unstable. The predominance of prismatic slip is a consequence of the initial CRSS ratios we used for prismatic : pyramidal : basal is 1 : 11.1 : 11.8, which, as mentioned, have been shown to well represent the plastic deformation of Zr [32]. The orientational instability found for over most of the orientation space is a result of the pronounced CRSS anisotropy characteristic of Zr.
5. Orientational stability of Zr/Nb bicrystals

The results from the spin-rate analysis, while in agreement with observations of rolled coarse-grained Zr, are, however, in significant contrast with the texture development seen in the nanolayered Zr, where the opposite result holds: the orientations covering Zr2, Zr3, Zr5, Zr6, and Zr7 are largely orientationally stable, and Zr1 and Zr4, are not.

The change in the orientational stability of a Zr crystal as it reduces from micron to nanoscale dimensions could have been induced by the increasing constraint with the neighboring Nb crystals. Across the Zr/Nb interface, the adjoining Nb and Zr nanocrystals must co-deform. Nb is much less plastically anisotropic than Zr and deforms by substantially many more slip systems. It
is possible that the nanograinaged Zr, when made to co-deform with a neighboring nano-grained Nb, can be brought into an orientationally stable state. Whether this happens would depend on the Nb crystal orientation and hence in this way, the Nb crystal could have provided the bias toward stability of Zr2, Zr3, Zr5, Zr6, and Zr7 over the other common rolling components.

To analyze the effect of Nb co-deformation on the orientational stability of Zr, we simulate the rolling of several Zr/Nb bicrystals. The preferred crystal orientations in the texture of the nanolayered Nb phase were selected for this purpose. In conventional rolling of BCC metals, two main fibers develop, the $\alpha$ and $\gamma$ fiber [68, 69]. Figures 6 and 7 display pole figures and the plots of the two fibers for three different layer thicknesses $h = 106 \, \mu m$, 92 nm and 41 nm [22]. Both fibers are seen to develop in the Nb phase, provided that the layer thicknesses of Nb were above 100 nm. The fiber plot for the $h = 106$ micron composite shown in Fig. 7 provides a typical example. However, as the Nb layers refine below 100 nm from 92 nm and then to 41 nm, the $\alpha$ and $\gamma$ fiber intensify with peaks forming around $\{111\} \langle 1\overline{1}0 \rangle$, $\{334\} \langle 1\overline{1}0 \rangle$ and $\{001\} \langle 1\overline{1}0 \rangle$, with a narrow +/- 5° deviation. The five main Nb orientations are listed on Table 1 and depicted in Fig. 8.
Figure 6 Pole figures showing the deformation texture in the Nb phase of the rolled Zr/Nb composite to (a) 106 μm, (b) 92 nm and (c) 41 nm layer thickness.
Bicrystals were created by considering all combinations of these five Nb orientations and the seven Zr orientations in Table 1. Figure 9 shows the model set up of the Zr/Nb bicrystal and the mesh used. The FE mesh consists of 3300 C3D8 (continuum three-dimensional eight-nodal) elements, which are divided into two equal sections representing individual single crystals of Zr and Nb. We use periodic boundary conditions [70], wherein the deformation of each pair of boundary faces (top/bottom, front/back and left/right) is equal and as a result the stress tensors on each pair are opposite in sign. The PSC boundary conditions are prescribed by specifying the displacement along the negative z-direction, while enabling the model to expand in the positive x-direction and keeping the y-dimension of the model constant during the deformation. These represent mixed boundary conditions that permit a non-zero rigid spin, which are more accurate, particularly for coupled bicrystals, than pure plane strain compression boundary conditions that would overconstrained the system by enforcing zero rigid spin.

**Figure 7** Fiber plots for the Nb phase in the Zr/Nb ARB composites with nominal at 106 μm, 92 nm and 41 nm layer thickness.
Figure 8 \{111\} pole figure showing location of the five Nb components studied in this work.

The same thermally activated dislocation density based hardening law used for Zr was employed for Nb, with, however, the specific slip modes and material parameters pertaining to Nb. The material parameters for \{110\}(1\overline{1}1) and \{112\}(1\overline{1}1) slip in Nb were characterized previously in [32] and these are the ones used here.

Figure 9 FE model consisted of 3300 C3D8 elements used in the DD-CPFE bicrystal simulations.

For assessing orientational stability, the Zr/Nb bicrystal simulations are used to analyze the c-axis lattice reorientation during rolling and 3D reorientation contours after 50% reduction. To
establish a connection with the underlying deformation mechanisms, we then study the relative contributions of slip associated with each case.

For all bicrystal combinations, Figure 10 presents the reorientation pathways taken by the c-axis of the Zr crystal on basal pole figures as the bicrystal is deformed up to 50% rolling reduction (approximately 60% strain). The pathway shown is the average over all points in the crystal. The darker colored points are the starting orientation and the lighter color points follow the reorientation path with strain. The color shades are divided into strain increments of 0.2. In nearly all the cases, the Zr crystals reorient away from their initial orientation toward the TD. They appear to be even less orientationally stable when constrained to deform with the Nb crystal. The only exceptions are the Zr1/Nb1 and Zr4/Nb1 bicrystal combinations; however, these two Zr orientations were not predominant in the nanolayered composites. Therefore, the compatibility constraint imposed by co-deforming with the Nb crystal neither stabilizes the Zr crystal nor does it choose to co-deform in a stable manner with a particular Zr component.
Figure 10 Basal pole figures for all 7 Zr and all 5 Nb orientations calculated based on the coarse-grained Zr slip resistance ratio: prismatic : pyramidal : basal = 1 : 11.1 : 11.8.

For more detail, Figure 11 compares the reorientation contours of the bicrystals at 0.6 strain. Again we see that the Zr4/Nb1 is stable with low total reorientation. The Zr1/Nb1 bicrystal, although undergoing minimal average reorientation, develops orientation gradients. Even more outstanding finding from these contours is that most of the Nb crystals remain relatively stable, experiencing little reorientation. The orientational stability of Nb is influenced negligibly by Zr, an outcome that likely is a consequence of its large number of slip systems and the relatively low differences in the CRSS values of \{110\} and \{112\} slip. Nonetheless, despite the stability of Nb and the kinematic constraint enforced by co-deformation between the Zr and Nb crystals, the Zr
is still orientationally unstable. Thus, the predominance of the Zr orientations, Zr2, Zr3, Zr5, Zr6, and Zr7, has little to do with its co-deformation with Nb.

Figure 11 3D reorientation contours for all 7 Zr and all 5 Nb orientations calculated based on the coarse-grained Zr slip resistance ratio: prismatic : pyramidal : basal = 1 : 11.1 : 11.8.

To relate texture evolution with the relative amounts of slip, we calculate from the model the relative activities of the three slip modes, basal, prismatic, and pyramidal slip. At an integration point at a given time (or strain) increment, we define the relative activity (RAα) as:

\[ RA^\alpha = \frac{\sum_s \dot{\gamma}_s^\alpha}{\sum_s \dot{\gamma}_s^B} \]  \hspace{1cm} (8)

For analysis, the relative activity RAα for a particular mode is then averaged over all integration points for every element.

Figure 12 shows the relative slip activities of the three modes in the Zr crystal during deformation. In nearly all cases, prismatic slip prevails, particularly near the end of deformation. The only exceptions lay in the two more orientationally stable bicrystals, Zr1/Nb1 and Zr4/Nb1,
where pyramidal slip dominates. Basal slip contributes very little. Broadly, these results can be expected from the highly anisotropic CRSS ratios among these three slip modes (1:11.1:11.8), characteristic of Zr.

**Figure 12** Relative activities associated with bicrystals for all 7 Zr and all 5 Nb orientations based on the coarse-grained Zr slip resistance ratio: prismatic : pyramidal : basal = 1 : 11.1 : 11.8.

6. **Reduced plastic anisotropy: orientational stability of Zr and Zr/Nb bicrystals based on the nano-grained CRSS ratio**

We consider next the second possibility that the highly oriented texture arises from a change in the slip activity resulting from a change in the activation of slip within nanocrystalline Zr. The prior set of CRSS values was based on the relative differences in activating and propagating prismatic, pyramidal, and basal slip dislocations in coarse-grained polycrystalline Zr. In these cases, the CRSS values are controlled by defects lying within the crystal interiors. In the present case, the Zr crystals are bounded by Zr/Nb interfaces and substantially less grain boundaries or
surfaces. The Zr/Nb interfaces will then serve as the primary sites for nucleation, annihilation sites, and barriers for slip. The change in slip activity could occur because the critical stresses for activating the various types of dislocations from the interfaces are not as disparate. Once nucleated, dislocations can glide unhindered to the other interface. On this basis, it is also possible that the critical resistance to dislocation motion is dominated by the nano-scale mean free path between adjacent interfaces. Consequently the differences in CRSS values among the three slip modes could have been reduced.

To relate a reduction in the plastic anisotropy of Zr to the evolution of crystal orientation in rolling, we adjust the initial CRSS ratios among prismatic : pyramidal : basal slip to be nearly unity to 1 : 1.8 : 1.12 in the hardening law. Although these CRSS ratios differ substantially from that characterized previously for coarse-grained Zr, it is fundamental to note, however, that prismatic slip still remains the easiest slip mode.

6.1. Spin-rate analysis

To determine the effect of reduced anisotropy on orientational stability, we first repeat the plastic rate analysis on single crystal Zr with the reduced CRSS ratios. Figure 13 shows the corresponding \( \dot{\theta} \) contour map. The striking difference from the analysis with conventional CRSS values is that all seven Zr crystal orientations are stable. This is a direct outcome of the substantially reduced anisotropy among the CRSS values. Thus less CRSS anisotropy, means more orientational stability.
Figure 13 Spin rate contours in Zr calculated based on prismatic : pyramidal : basal slip ratio of 1 : 1.8 : 1.12.

6.2 Bicrystal deformation with reduced anisotropy

The spin-rate analysis with reduced plastic anisotropy in Zr shows that the orientational stability of the seven Zr single crystals has substantially improved. When co-deforming with a Nb crystal, the orientationally stability can change. To better understand their development in the Zr/Nb nanolayered composites, we repeat the bicrystal simulations with reduced plastic anisotropy in Zr. We again consider a bicrystal consisting of all combinations of Zr and Nb orientations. Figure 14 shows the average c-axis reorientation pathways for Zr on basal pole figures. The most important finding is that by this metric the predominant components Zr2 and
Zr3 in the nanolayered composites are stable with all five Nb crystals. This result is a significant deviation from the behavior of Zr/Nb bicrystals in which Zr deformed using the conventional set of activation stresses. Most importantly it is consistent with the highly oriented Zr textures that develop in the nanolayered Zr/Nb composites, where it was seen that Zr2 and Zr3 should prevail over the other common rolling components in rolling.

![Figure 14](image)

**Figure 14** Basal pole figures for all seven Zr and all five Nb orientations based on the nano-grained (reduced anisotropy) Zr slip resistance ratio: prismatic : pyramidal : basal slip ratio of 1 : 1.8 : 1.12.

The paths taken by the Zr orientations, Zr5, Zr6, and Zr7, are shown in Fig. 14 columns 5, 6 and 7. Again, unlike the behavior of the Zr/Nb bicrystals with conventional CRSS ratios for slip, the bicrystals with Zr6 and Zr7 are orientationally stable. Zr5 is less so, but Zr5 reorients a small
degree from its initial position toward Zr6. In contrast to conventional anisotropic Zr and consistent with experiment, for reduced anisotropic Zr, orientations Zr6 and Zr7 are orientationally stable.

Last, we remark on the calculated reorientation paths for those Zr orientations not seen in the nanolayered Zr textures, Zr1 and Zr4, which are shown in Fig. 14, columns 1 and 4. We observe that the usually stable components in rolled single phase Zr, Zr1 and Zr4 are no longer stable when co-deforming with Nb and the anisotropy of Zr has been reduced. Not only are they unstable, but they are found to reorient towards Zr2 and Zr3, the preferred components seen in the highly oriented texture that develops in the nanolayered Zr/Nb composites.

Figure 14 displays the c-axis reorientation only. The average total reorientation angles for anisotropic and reduced anisotropic Zr are compared in Table 2. We see that reduced anisotropy in Zr has the most profound influence on stabilizing Zr2 and Zr3 in rolling, which strongly indicates that the unusual, highly oriented texture that emerges in the rolled nanolayered Zr phase is a consequence of reduced CRSS anisotropy.

<table>
<thead>
<tr>
<th>$\Delta \theta_{Zr}$[^°]</th>
<th>Zr1</th>
<th>Zr2</th>
<th>Zr3</th>
<th>Zr4</th>
<th>Zr5</th>
<th>Zr6</th>
<th>Zr7</th>
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<td>Nb1</td>
<td>8.8/4.5</td>
<td>20.8/1.5</td>
<td>17/0.6</td>
<td>0.8/0.3</td>
<td>23.3/9.6</td>
<td>19.7/7.8</td>
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</tr>
<tr>
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<td>14.3/0.8</td>
<td>24.6/16</td>
<td>22.1/10.6</td>
<td>19.9/6.3</td>
<td>24/1.2</td>
</tr>
<tr>
<td>Nb3</td>
<td>26.6/12.2</td>
<td>17.8/3.4</td>
<td>13.5/0.7</td>
<td>28.5/17.7</td>
<td>21.8/9.8</td>
<td>20.1/5.5</td>
<td>24.1/4.1</td>
</tr>
<tr>
<td>Nb4</td>
<td>28.7/11.7</td>
<td>17.8/3.1</td>
<td>13.2/0.6</td>
<td>31.5/17.1</td>
<td>22/8.4</td>
<td>19.8/4.2</td>
<td>24.7/9</td>
</tr>
<tr>
<td>Nb5</td>
<td>28.7/11.2</td>
<td>18.2/2.7</td>
<td>13.5/0.5</td>
<td>30.6/16.8</td>
<td>22.4/7.7</td>
<td>19.7/4.4</td>
<td>24.9/9.8</td>
</tr>
</tbody>
</table>

Table 2. Average reorientation angle over the FE mesh for individual Zr components at a strain of 0.6: conventional and reduced anisotropy Zr CRSS ratio.
For a more refined analysis of orientationally stability, Figure 15 presents the 3D reorientation contours of the Zr/Nb bicrystals after a certain amount of strain with the plastically low anisotropic Zr. As seen before in Zr/Nb bicrystals with conventional Zr CRSS values, the Nb remains stable during rolling. However, the compelling results lie in the behavior of the Zr crystal, which has changed substantially. First, compared to the single Zr crystal with the same reduced anisotropic CRSS values and orientation, the Zr crystal is less orientationally stable when joined to the Nb crystal. Thus, being bonded to Nb makes the Zr crystal less, not more, stable. Second, when bonded to the same Nb crystal, the Zr crystal with reduced anisotropy in slip reorients much less than the same Zr crystal with higher anisotropy. Last, when considering all five Nb crystals, bicrystals with Zr2 and Zr3 are the most stable and Zr1 and Zr4 are the least. Zr6 and Zr7 are orientationally stable for some Nb crystals, but not for others. In particular, when bonded to Nb3, Nb4, and Nb5, Zr orientation Zr7 develops orientation gradients. Thus, once again, consistent with the nanolayered Zr textures, these more highly resolved model calculations reveal that Zr2 and Zr3 are the most stable and should prevail over the other common rolling components in PSC, when co-deforming with Nb and the plastic anisotropy of Zr has been reduced.
Figure 15 3D reorientation contours for all seven Zr and all five Nb orientations based on the nano-grained (reduced anisotropy) Zr slip resistance ratio: prismatic : pyramidal : basal slip ratio of 1 : 1.8 : 1.12.

6.3 Relative activities

With the model, we can directly link texture evolution with the underlying slip activity. With reduced anisotropy and remarkable changes in which orientations prevail as stable, we cannot expect the slip patterns to be the same as those seen in conventional Zr.

Figure 16 presents the relative activities associated with bicrystals for all Nb and Zr with reduced CRSS anisotropy. A common feature of the more orientationally stable cases, Zr2 and Zr3, when joined with most of the Nb orientations (Nb2-Nb5), is that they deform by similar amounts of slip from all three slip modes. The same collaborative slip pattern is also seen in the other outstanding stable orientation, Zr6, when joined with Nb2-Nb5. Conversely, those lesser stable bicrystals, such as those including Zr1 and Zr4, the deformation is dominated by pyramidal slip. It is important to note that for every starting bicrystal orientation, the CRSS ratios for Zr were reduced, but only in a few orientations does this reduction result in orientational
stability in rolling. Most significantly, these few orientations are those seen experimentally in the highly oriented nanolayered Zr/Nb composites.

![Figure 16](image)

**Figure 16** Relative activities associated with bicrystals for all 7 Zr and all 5 Nb orientations calculated based on the nano-grained Zr slip resistance ratio: prismatic : pyramidal : basal slip ratio of 1 : 1.8 : 1.12.

7. Discussion

In this work, deformation texture evolution is used as a signature for inferring the types of slip patterns that dominate the plastic deformation of nanocrystalline Zr. With crystal plasticity, we predict that only when the CRSS ratios among prismatic, pyramidal and basal reduce substantially to values below 2, do the predominant Zr2 and Zr3 orientations seen in nanocrystalline Zr become stable in rolling while the other conventional rolling components Zr1 and Zr4 turn unstable. The reason for the reduce anisotropy, however, has yet to be clarified. It has been proposed in [71] that the reduction in CRSS differences among distinct slip modes occurs because in nanoscale crystals the CRSS has increased substantially above the friction
stress for all slip systems. As one possibility, the enhancement could arise from a significant reduction in the mean free path for dislocation glide as layers attain nanoscale dimensions. In a recent study on the ARB Cu/Nb nanolayered system, a continual strengthening with increased reduction in \( h \) down to at least \( h = 15 \) nm was reported and shown to follow a Hall-Petch-like law [72]. On this basis, we can consider hypothetically the situation in which the CRSS enhancement is due to the Hall-Petch strengthening only, \( \tau_{c-ng}^{\alpha} = \tau_{c-cg}^{\alpha} + K_{\alpha}/\sqrt{h} \), where \( \tau_{c-cg}^{\alpha} \) are the established CRSS values giving the macroscopic yield strength for coarse-grained Zr [32]. For \( h = 100 \) nm, the reduced anisotropic CRSS ratio of 1:1.8:1.1 can be estimated using \( K_{\text{prism}} = 230 \) MPa \( \mu \text{m}^{1/2} \), \( K_{\text{pyr}} = 385 \) MPa \( \mu \text{m}^{1/2} \) and \( K_{\text{bas}} = 220 \) MPa \( \mu \text{m}^{1/2} \). The resulting nano-grained, \( \tau_{c-ng}^{\alpha} \), values are 750 MPa, 1350 MPa, and 840 MPa for prismatic, pyramidal and basal. These values produce a material yield stress that is consistent with the hardness value of 4.5 GPa measured for this nanocomposite.

It may also be the case that the CRSS enhancement arises because the CRSS is associated with the barrier for nucleating dislocations from interfaces rather than the resistance to motion across a forest of dislocations accumulated the crystal. To obtain the ideal values for producing and moving dislocations, we calculated using first principles DFT the generalized stacking fault energy (GSFE) curves on the prismatic, basal, and pyramidal I slip system.

The DFT calculations were performed using the VASP code [73, 74]. In these calculations, a pseudopotential is employed to model the interaction between the valence electrons and ionic cores. For the exchange correlation functional in DFT, we adopted the generalized gradient approximation (GGA) with the Perdew-Becke-Erzenhof (PBE) parameterization [75]. The number of valence electrons in our Zr pseudopotential is four. To obtain the (GSFE) curves for a given slip (x-z) plane, the upper half of the crystal is shifted rigidly with respect to the lower half.
in the z-direction. Atoms are free to relax in the x and y directions. All the calculations were performed with periodic boundary conditions and with an energy cutoff of 400 eV for the plane wave expansion within the projector augmented wave (PAW) formalism [76, 77]. We used the gamma centered Monkhorst-Pack [78, 79] k-point mesh with a Gaussian smearing for the Brillouin zone integrations. The k-point mesh was large enough that the convergence of total energy was less than 1 meV per atom with respect to change in k-point mesh size. An optimized structure was obtained when the force on each atom is smaller than 0.01 eV/A. The calculated ⟨a⟩ and ⟨c⟩ lattice parameters for the Zr primitive unit cell are 3.231 Å and 5.174 Å, respectively, which agrees well with experimental measurements [80] and earlier calculations [81].

Figure 17 shows the calculated GSFE curve for the prismatic slip system. This energy profile shows a very weak local minimum so dissociation of full dislocation into the partials is not stable and thus, unlikely. The peak value, or the unstable stacking fault, γusf, can be related to the barrier to produce the dislocation. The lattice resistance can be also estimated from the γ surface by the maximum value of (1/b)dγ/du [82]. For the prismatic dislocation, γusf = 202 mJ/m² and the lattice resistance is 2.4 GPa.

For comparison, Fig. 17 also shows the GSFE curve for the basal plane {0001} in the direction of the Burgers vector for a full dislocation 1/3 ⟨11̅20⟩. For the full basal dislocation, γusf = 273 mJ/m² and the lattice resistance, 3.5 GPa, which are higher than those for prismatic.

Last, the GSFE curve for pyramidal type I slip is provided in Fig. 17. Two local minima develop, suggesting that the dislocation can reduce its energy by dissociating into partial dislocations. The γusf and lattice resistance from the maximum of (1/b)dγ/du are taken from the sense of direction where both are lower (from right to left in Fig. 17) and these are 479 mJ/m² and 5.2 GPa, respectively.
Figure 17 DFT calculated GSFE curves for the prismatic, basal, and pyramidal slip systems for Zr. The displacement on the x-axis is normalized by the corresponding full dislocation Burgers vectors.

Taken together, we find that the ratios of the $\gamma_{usf}$ from prismatic : pyramidal : basal are 1:2.37:1.35 and for the resistance they are 1:2.17:1.45., notably comparable to the CRSS ratios (1:1.8:1.12) found via crystal plasticity for the nanolayered Zr material and substantially reduced from the CRSS ratios characteristic of coarse-grained Zr (1:11.1:11.8).

8. Conclusions

In this work, we use a 3D multiscale crystal plasticity based model to study the orientational stability of nanocrystalline Zr in rolling. The material studied is nano-layered Zr/Nb composites made by accumulative roll bonding. It was reported that once the layers reduced below 100 nm, the texture became unusually highly oriented in a few special orientations. Thus, the nanolayered Zr phase provided the opportunity to study potentially unconventional aspects of plastic deformation of nanocrystalline hcp Zr as well as the effects of co-deformation between the Zr/Nb nanocrystals. Other SPD methods on single-phase Zr cause phase transformations or are unable to refine hcp Zr to very fine nano-grain dimensions.
The rolling deformation simulations are carried out on both single crystal Zr and Zr/Nb bicrystals. The analysis finds that Zr crystals, when bonded to Nb crystals become less orientationally stable than the same single crystal orientation under the same deformation state. We show that conventional plastic anisotropy characteristic of coarse-grained Zr leads to stable texture components that deviate from those that emerge in the nanolayered composites. A substantial reduction in the CRSS ratios among the slip modes below 2 causes the few observed texture composites in nanolayered to become stable at the expense of the instability of the more common components. The few special Zr orientations that prevail under reduced anisotropy involve nearly equal contributions of all three slip modes. This slip pattern is shown to be significantly different than that operating in coarse-grained Zr. These results thus strongly suggest that the differences in activation stresses for slip in nanograined Zr are significantly lower than that of coarse-grained Zr. The near equalization of the critical stresses for activating slip is attributed to a transition from crystal-controlled to interface-controlled dislocation nucleation and propagation. Using DFT, we show that the reduced CRSS ratios among the three slip systems are consistent with the stresses required to form these dislocations. Although we focus this study on nanocrystalline Zr, the findings are sufficiently general to provide insight into mechanisms underlying the nanotrusturcuring SPD processes of other hcp metals.

Acknowledgements
This work is based upon project supported by the National Science Foundation under grant No. CMMI-1541918. The authors gratefully acknowledge this support. IJB and AK would like to acknowledge support through a Los Alamos National Laboratory Directed Research and Development (LDRD) project ER20140348.
Appendix A.

Table A1 shows 12 equivalent crystal orientations within the rotational point symmetry group associated with HCP crystals.

<table>
<thead>
<tr>
<th>Symmetries 1–4</th>
<th>5–8</th>
<th>9–12</th>
</tr>
</thead>
<tbody>
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<td>((\varphi_1, \Phi, \varphi_2))</td>
<td>((\varphi_1, \Phi, \varphi_2 + \frac{\pi}{3}))</td>
<td>((\varphi_1, \Phi, \varphi_2 + \frac{2\pi}{3}))</td>
</tr>
<tr>
<td>((\varphi_1, \Phi, \varphi_2 + \pi))</td>
<td>((\varphi_1, \Phi, \varphi_2 + \frac{4\pi}{3}))</td>
<td>((\varphi_1, \Phi, \varphi_2 + \frac{5\pi}{3}))</td>
</tr>
<tr>
<td>((\varphi_1, \Phi + \pi, \varphi_2))</td>
<td>((\varphi_1, \Phi + \pi, \varphi_2 + \frac{\pi}{3}))</td>
<td>((\varphi_1, \Phi + \pi, \varphi_2 + \frac{2\pi}{3}))</td>
</tr>
<tr>
<td>((\varphi_1, \Phi + \pi, \varphi_2 + \pi))</td>
<td>((\varphi_1, \Phi + \pi, \varphi_2 + \frac{4\pi}{3}))</td>
<td>((\varphi_1, \Phi + \pi, \varphi_2 + \frac{5\pi}{3}))</td>
</tr>
</tbody>
</table>

Table A1. Twelve symmetry operations within the hexagonal close packed (HCP) rotational point symmetry group.

Appendix B. Supplementary data

The following are the supplementary data to this article:

1. All three poles for Zr5 with all the 5 Nb orientations with the conventional and reduced anisotropy CRSS values at a strain of 0.6

![Images of pole figures for Zr5 with Nb orientations at different strains]
All three pole figures for Zr crystal orientation Zr5 with all five Nb orientations (coarse grained, conventional CRSS ratio).

2. All three poles for Nb1 and Nb2 with all the 7 Zr orientations for the reduced anisotropy CRSS at a strain of 0.6.
All three pole figures of Nb orientation Nb1 with all seven Zr orientations (nano grained, reduced anisotropy CRSS ratio).

All three pole figures of Nb orientation Nb2 with all seven Zr orientations (nano grained, reduced anisotropy CRSS ratio).

References


Chapter 5

This chapter is currently under review with a title: Room temperature deformation mechanisms of Mg/Nb nanolayerd composites, Milan Ardeljan, Manish Jain, Siddhartha Pathak, Anil Kumar, Nan Li, Nathan A. Mara, Kevin J. Baldwin, Marko Knezevic, Irene J. Beyerlein, Materials Research Society (submitted). My role in preparing this chapter was to numerically implement the confined layer slip (CLS) model into CPFE, which greatly contributed to fundamental understanding of how Magnesium-Niobium nano-layered composites deform elastically and plastically at nanometer length scales. I designed and generated appropriate finite element microstructures that realistically correspond to different layer configurations of MgNb micro-pillars. I performed the modeling work, necessary to determine both elastic and plastic behavior of the composite using CPFE framework, post-processing of the relevant data and generating corresponding figures. I also provided written descriptions of all the developed procedures.
Room temperature deformation mechanisms of Mg/Nb nanolayered composites

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Abstract

The goal of this work is to gain an understanding of the deformation mechanisms underlying the room temperature deformation of the bcc Mg phase in nanolayered composites. Nanolayered composites comprised of 50% volume fraction of Mg and Nb are made via physical vapor deposition with individual layer thicknesses h of 5 nm and 50 nm. We use a combination of DFT for relative barriers to shear on crystallographic slip systems and Mg/Nb interface, and a novel model that implements CLS into a CPFE code for the deformation of nanolayers. Calculations from a multiscale crystal plasticity finite element model predict that the stress-strain response results from dislocation mediated plasticity on the \{110\}\{111\} and \{112\}\{111\} slip systems and no twinning. At h = 5 nm, the Mg has undergone a phase transition from HCP to BCC such that it forms a coherent interface with the Nb phase. A CP model with the h dependent CRSS is developed and applied to understand the linkage between the observed deformation response and underlying mechanisms.

KEYWORDS
Dislocations, crystallographic structure, nanostructure, strength, phase transformation
1. Introduction

Interface strains can change the phase of a metal from its stable form in ambient conditions\(^1\). Of the two dissimilar metals that are joined at their common interface, one metal can adopt the crystal structure of the other\(^1\). Many examples include nanolayered bimetal composites, which consist of alternating nanoscale thick layers of two metals, which are immiscible in ambient conditions\(^2-8\). To induce the phase transformation, the individual layer thicknesses must be sufficiently fine, usually on the order of a few nanometers. This strategy has been exploited to form bcc Zr by joining conventional hcp Zr to bcc Nb or the formation of fcc Ti, when Ti is joined with fcc Al or Ag, and bcc Mg when hcp Mg is joined with bcc Nb\(^9\). These are just some of the many examples that can be found in the literature. These studies have shown that the pseudo-morphic phases exhibit unusual properties not familiar to its original stable state, such as a decrease in the superconducting transition temperature\(^10\). The structural properties of these materials have not been thoroughly studied, however. One exception is the work of Zhang et al.\(^11\) on fccCu/fccNb, who found that the composite with the metastable fcc Nb phase was stronger than the FCC/BCC Cu/Nb composite for the same layer thickness. The origin of the strengthening effect of the fully FCC composite was unknown since the composite differed in other microstructural aspects such as grain shape and interface type. Nanolayered composites with new interface-induced phases can give rise to new possibilities for the deformation mechanisms and properties of the composite.

With the introduction of micropillar testing, it is possible to test the deformation response of micron-diameter and nanoscale diameter pillars made from thin films\(^12-15\). This technique has been used over the years to study the elastic and inelastic responses of nanolayered composites comprised of phases in stable state at ambient temperatures and pressures\(^16,17\). It has been shown
that these bimetal nanolayered composites can possess extraordinarily high strengths when the individual layer thickness is decreased down to 5-10 nm, several times larger than a simple volume average of the strengths of the constituents\textsuperscript{13, 14, 16, 17}. Equal volume fraction (50/50) Cu/Nb nanolayered composites, for instance, are found to be much stronger (5X) than a strength calculated from rule-of-mixtures of their phases and much more thermally stable, shock resistant, and radiation resistant than Cu alone\textsuperscript{14, 18-23}. Likewise, 50/50 Zr/Nb nanolayered composites are much harder and stronger than bulk Zr and bulk Nb alone\textsuperscript{24}. Further, when combined with transmission electron microscopy, they can reveal evidence of deformation and failure mechanisms, such as interfacial sliding, confined layer slip, twinning, and cracking\textsuperscript{25-28}.

These techniques are not often used to study properties of nanolayered composites with pseudo-morphic phases. Recently, it was demonstrated by testing of micron-sized pillars of MgNb layered composites that the bccMg/Nb composite was 50% stronger and the strain to failure 36% larger than the hcpMg/Nb nanocomposite\textsuperscript{29}. For Mg, the difference marked an outstanding result from a technological point of view. While hcp Mg is attractive due to its lightweightness and abundance, it has low strength and ductility relative to other commonly available metals like steel and aluminum alloys. One of the main reasons for its poor formability concerns the low symmetry HCP crystal structure, which leads to a pronounced sensitivity of its plastic behavior to loading direction, temperature and strain rate\textsuperscript{30-37}. Usually the critical stresses to activate slip in the \langle a \rangle direction are several times smaller than those in the \langle c + a \rangle direction\textsuperscript{38, 39}, so crystals oriented well for predominant \langle a \rangle slip activity deform under less stress than those oriented well for predominant \langle c + a \rangle slip activity. The bcc crystal structure, on the other hand, is more symmetric and has at least 48 available slip systems with similar activation stresses and hence generally more ductile than hcp metals.
One of the issues in determining the mechanical properties of pseudo-morphic phases is that many of the basic deformation mechanisms of the new phase are not known. In addition, the observed differences in strength between the stable phase and metastable pseudo-morphic phase could not be easily attributed to the pseudo-morphic phase change alone. In the case of the Mg/Nb example above, the two nanolayered composites, the 5 nm bcc Mg/Nb and 50 nm hcp Mg/Nb composites, had many microstructural differences, such as layer size, grain aspect ratio, crystal structure, potential slip and twinning systems, crystallographic texture, and interface type.

In this work, we investigate the elastic and plastic properties of a nanolayered Mg/Nb composite. Thin film composites were made via physical vapor deposition (PVD) with alternating nanoscale layers of Mg and Nb with equal thickness h. Sample layer thicknesses h were either at or above the critical transition layer size (~5 nm), so that one contained only hcp Mg and the other only bcc Mg. Micropillar compression tests were carried out in two different directions, normal to the layers and parallel to them. To gain some insight into mechanisms, DFT calculations on ideal shear strengths of the possible glide systems and interfaces in bcc Mg were carried out. The information is used to build a multiscale CPFE model with texture evolution and layer size-dependent slip systems via a confined layer slip (CLS). It is applied to both the hcp Mg/Nb and bcc Mg/Nb nanostructures to simulate compression in the parallel and normal layer directions. The results indicate that the strengthening observed in the bccMg composite over the hcpMg composite were not due to the effects of the change in interface type. In fact, the analysis suggests that the interface/dislocation interactions on the resistance to confined layer slip are found weaker in the coherent bccMg/bccNb interface compared to the hcpMg/bccNb interface. The analysis revealed that the key contributions of strengthen of the bcc Mg composite
are predominantly reduction in layer thickness \( h \) from 50 nm to 5 nm and intrinsically harder \{110\} and \{112\} slip in bcc Mg than basal slip in hcp Mg.

2. Interface-induced phase transformation

In a layered composite, the phase transformation results from a balance of interface energy and bulk energy\(^1,40,41\). A rough approximation of the critical layer thickness to transform Mg from its stable hcp form to its bcc form can be obtained by comparing the total energy with an hcp Mg layer and an bcc Mg layer. The total energy of the system per unit area is comprised of the elastic energy resulting from the coherency strains, the cohesive energy in each phase, and the interface energy, i.e.,

\[
E_{\text{tot}} / A = h_{\text{Mg}} (E_{\text{Mg}}^{\text{elas}} + E_{\text{Mg}}^{\text{bulk}}) + h_{\text{Nb}} (E_{\text{Nb}}^{\text{elas}} + E_{\text{Nb}}^{\text{bulk}}) + 2\gamma,
\]

where \( h_{\text{Mg}} \) and \( h_{\text{Nb}} \) are the layer thicknesses for the Mg and Nb phase and \( \gamma \) is the interface energy. The calculation is performed separately for the 50/50 HCP Mg/ BCC Nb and HCP Mg/BCC Nb systems, as a function of their common h value. The interface energies for a coherent BCC Mg/BCC Nb and semi-coherent hcpMg/BCC Nb interfaces were obtained from DFT to be 304 mJ/m\(^2\) and 624 mJ/m\(^2\), respectively\(^41\). For the elastic energy, it is assumed that under no applied strain or pressure, the elastic strains are solely the result of coherency strains generated at the coherent Mg/Nb interface. With these values inserted into eqn (1), the model predicts that the critical Mg layer thickness \( h \) for 50/50 Mg/Nb composite, at which the total energy with the coherent bcc Mg phase exceeds that of the hcp Mg phase is 4.2 nm. These results are not too different than the 5 nm value predicted for the same 50/50 composite by more sophisticated thermodynamic calculations carried out by Junkaew et al.\(^40\)
Based on this prediction, nanolayered 50/50 Mg/Nb composites were made with an individual layer thickness of roughly 5 nm, another of 6.7 nm, and last, 50 nm. These nanolayers were prepared using the hybrid sputtering-evaporation PVD chamber (AJA International, Inc.). Both Mg and Nb layers were deposited in a magnetron sputtering system with a base pressure of 2×10⁻⁸ Torr. Both layers were deposited using DC magnetron sputtering at a process pressure of 3 millitorr with 300 watts of power on a 2-inch target. The deposition rates were 0.83 nm/sec for Mg and 0.22 nm/sec for Nb. The total film thicknesses for all samples were approximately 10 µm. To minimize residual stresses, several substrate materials (MgO and Si) and orientations were considered. The substrate material leading to the smallest residual stresses was Si in the (001) orientation and this was used for all samples studied here.

XRD analysis is used on the deposited nano-composites to determine the present crystal structure of Mg (hcp vs. bcc), as well as for texture measurement. XRD results indicate that Mg in the 50 nm Mg/Nb nanocomposites is in its traditional hcp structure, while for the lower layer thicknesses of 5nm Mg has undergone an interface strain induced phase transition from hcp to bcc structure.

XRD analysis is also employed on all samples for texture measurement. Textures were measured on both the top or bottom surfaces of the samples using a Bruker/AXS diffractometer equipped with a General Area Detector Diffraction System (GADDS) area detector at the University of New Hampshire, using Co-Kα radiation (operating at 40 kV and 20 mA) and a graphite incident beam monochromatic was used to eliminate the Kβ line. The beam was collimated to a spot size of ~1.0 mm. The Matlab toolbox software MTEX⁴² was utilized to reconstruct the orientation distribution functions (ODF) from the measured XRD pole figures.
with the crystallite orientation densities in a three-dimensional orientation space defined by the Bunge-Euler angles $\phi_1$, $\Phi$ and $\phi_2$.

Figure 1 shows the measured XRD textures for the 50 nm and 5 nm samples. In all cases, the texture is strong and axisymmetric about the normal direction (ND). For the 50 nm composite, the basal poles in the HCP Mg phase are highly aligned along the ND of the film. In the BCC Nb phase in this composite, the $\{011\}$ poles are oriented along the ND. In the 5 nm and 6.7 nm composites, texture measurements show that the textures of the bcc Mg and bcc Nb phase textures are identical and very similar to the Nb phase texture in the 50 nm composite. These textures are consistent with prior microstructural analyses of fully bccMg/Nb composites\textsuperscript{40,43,44}. In these other works, however, the 5 nm/5 nm Mg/Nb composite was not fully bcc. Finer h to 2.5 nm (with Nb at the same h) or 1.5 nm (with Nb at a smaller h) was needed to create the fully bccMg/bccNb composite.
Figure 1 Initial pole figures of the XRD measured textures of (a) HCP Mg (50 nm) and (b) BCC Nb (5 nm and 50 nm) and BCC Mg (5 nm). At 5 nm layer thickness BCC Nb and BCC Mg have the same initial texture.

The Mg/Nb interface plane normals are nominally parallel to the film axis. The bulk texture result suggests that the nanocrystalline HCP Mg and BCC Nb phases are joined at an interface with their \{110\}//\{0001\}. In the 5 nm and 6.7 nm composites, the BCC Mg and BCC Nb phases sharing the same orientations, and from this, it would be expected that the bcc Mg/bcc Nb interfaces are cube-on-cube, with all crystallographic planes and directions aligned on either side of the interface.

A closer look at the interface in these two types of samples is done via TEM analysis. The TEM images of layered material and HR-TEM images of one typical interface are presented in figure 2. The 50 nm hcp Mg/bcc Nb forms an interface that joins the \{0001\} Mg plane with the \{110\} Nb plane. The \{1120\}Mg is aligned with the \{111\}Nb. This crystallographic character would be associated with a semi-coherent interface, described by a network of misfit dislocations separated by coherent interface. The 5 nm bcc Mg/bcc Nb forms a coherent, cube-on-cube
interface. They are joined at their mutual \{110\} planes. This crystallographic interface character is similar to those found in other fully coherent bccMg/bccNb composites made by PVD reported in the literature\textsuperscript{40,45}.

![HR-TEM images](image)

**Figure 2** HR-TEM images taken of the (a) 50 nm/ 50 nm HCP Mg/BCC Nb and (b) 5 nm/5 nm BCC Mg/BCC Nb. Taken with permission from\textsuperscript{29}.

To determine the effect of layer thickness on strength, indentation hardness measurements were made on the three samples made. Figure 3 shows the results on a Hall Petch plot. The hardness is outstandingly higher, over 10 times that of coarse-grained Mg or Nb or approximately 2-3 times that of nanocrystalline Mg or Nb\textsuperscript{45,46}. Another important finding is that hardness is sensitive to h, continually strengthening as h decreases. Compared to prior results on PVD films\textsuperscript{43} these hardness values are 47\% higher. As mentioned, in the prior work, the Mg phase in the composites were not fully bcc Mg until h < 5 nm.
3. Deformation response

To investigate the effect of the phase on the deformation properties, micropillar compression tests were carried out on the 5 nm and 50 nm 50/50 Mg/Nb nanolayered composites. The FEI Helios FIB located at CINT-LANL (EML) was used to fabricate two types of micro-pillars from the PVD foils, one in which the Mg/Nb interfaces are aligned normal to the loading direction and another in which they are parallel to it. In situ SEM micro-pillar compression tests were then performed on these FIB’ed samples using the Hysitron PI-85 in the Magellan SEM.

3.1 Normal to the interfaces

Figure 4 presents a few stress-strain curves for each sample in the case in which the interface normal is aligned with the loading direction (see inset in figure 4). Identical tests produced nearly the same curves, confirming outstanding repeatability. Comparing the two samples, the results revealed that bcc Mg in a nano-composite is 50% stronger and has a higher strain to failure than
its hcp counterpart (see figure 4). In-situ observation during the compression tests show that the 50 nm Mg/Nb nanolayered composite failed by shear localization, whereas the 5 nm Mg/Nb did not. In the former, when the peak stress is reached, a shear band has already formed in the lower half of the pillar and propagated across the diameter.

![Figure 4](image_url)

**Figure 4** Comparison of stress-strain response between Mg/Nb 5nm/5nm and 50nm/50nm multilayered nanocomposites with interfaces oriented normal to the loading direction. SEM images at yield and after instability are shown.

Post-mortem TEM analysis was carried out on the samples after deformation. The FIB lift-out technique was applied to prepare the TEM foils from compressed pillars. Foil location was taken from the middle of the pillar. The final cleaning step was performed with beam current of ~50 pA and a voltage of 8 keV, in which FIB induced damage is minimized. The microstructure has been probed using an FEI Tecnai F30 field emission gun TEM. Figure 5(a) shows the
deformed 50 nm HCP Mg/BCC Nb pillar. The dark layer corresponds to Nb and light layer corresponds to Mg phase. A shear band has been developed when the strain goes beyond 10%. The nominal plane of the shear band is closely aligned with Mg (1124) plane. The average bilayer thickness has been measured as a function of the distance to the substrate. At top region of the pillar, the average bilayer thickness has the minimum value and uniform compression deformation occurs. At the edge of the pillar, there is no indication of Mg phase being extruded out. The Mg and Nb phase co-deform: the Mg phase is thinning relative to the Nb phase. No deformation twins were found from TEM analyses made after these tests. Pure Mg, as a coarse-grain polycrystal, is known to deform by slip and deformation twinning, and to have limited ductility and small strains to failure in compression, e.g., < 10%. Nanoscale hcp Mg, however, does not twin as readily, and could have larger strains to failure than coarse grained Mg. Thus, the observation of slip-dominated deformation in both present types of composites is consistent with prior reports of nanoscale hcp Mg. For comparison, Figure 5(b) shows an image taken of the bcc Mg/Nb pillar after failure. The morphology of three different locations (top, middle and bottom of the pillar) has been magnified, and the correlated average bilayer thickness has been measured and plotted on the left. The key observations are the co-deformation of the Mg and Nb phases and no deformation twinning. Taken together, the analysis suggests that the nanocomposite deformation was dominated by crystallographic slip in the layers.
Figure 5 TEM images after deformation of (a) the 50 nm HCPMg/BCCNb pillar and (b) the 5 nm BCCMg/BCCNb pillar.

3.2 Parallel to the layers

Figure 4 also shows the stress strain curves measured from micropillar testing parallel to the layers. For both composites, the flow stress in the layer-parallel load direction is lower than in the layer-normal direction. As in the normal loading test, the flow response of the bcc Mg/Nb composite is higher than that of the hcp Mg/Nb composite. The notable differences are that the strength difference is not as great in parallel direction as in normal direction (peak stress of 1.6 GPa vs 1.4 GPa). Also, the compression strain to reach the peak stress is nearly the same (~0.04). Lastly, the plastic anisotropy as measured by the difference in the layer parallel and normal cases
for the same composite is higher in the bccMg/Nb case than the hcpMg/Nb case. This last aspect may be counterintuitive as bcc metals typically are less plastically anisotropic than hcp metals.

In the 50-50 nm composite, the softening occurred due to the onset of kink banding. The fully developed kink band can be seen at the bottom of the pillar in Figure 4(d). In the 5-5 nm composite, pronounced softening did not occur and no kink bands were observed. These results are in contrast to prior layer parallel compression tests on ARB Cu-Nb nanolayered composites\textsuperscript{50}. Samples of all layer thicknesses from \( h = 15 \) to 250 nm failed by kink banding and the finer \( h \), the lower the strain to initiate kink banding. It was proposed that the strongly textured layers lead to the highly anisotropic properties of this material, which is a characteristic of materials that tend to fail by kink banding\textsuperscript{51}.

4. Deformation mechanisms

Knowledge of the deformation mechanisms are critical for understanding the various aspects in the flow responses of these two materials, bearing different crystal structures of Mg, and for potential employment of pseudo-morphic phase based materials in structural applications. The decreasing strain hardening rate with strain in each curve suggests that the curves were mediated by dislocation glide. As further support, the TEM analysis of the samples deformed in compression normal to the layers did provide evidence of co-deformation and did not provide evidence of twinning.

From the TEM analysis and micropillar tests alone, however, knowledge on the operative mechanisms underlying the observations is limited. Furthermore, the two materials tested here differ in many aspects-not just the crystal structure of the Mg phase-that can affect dislocation motion, and hence strength and deformation flow response. They differ in elastic modulus, lattice parameter, layer size (5 nm vs 50 nm), slip modes, grain shape (aspect ratio of 1:2 vs 1:20),
interface structure (coherent vs semi-coherent) and texture. To complement the effort towards understanding the deformation mechanisms in bcc Mg, we carry out DFT and crystal plasticity calculations.

The crystal lattice and electronic structure determine the elastic modulus, and crystallographic planes and directions on which dislocations move and their relative resistances. Layer size can also affect dislocations, particularly when size scales are within an order of magnitude of the core of the dislocation (few nm). It has been discussed in prior works that reducing the layer size can affect number density of sources or the ease of dislocation annihilation, and the stress to propagation\textsuperscript{52-59}. In nanolayered composites, the interfaces play a key role in the strength through their interactions with the moving dislocations and possibly nucleation and expanding twins\textsuperscript{60}. Many possible interactions have been proposed by theory and analytical modeling or observed in atomistic simulation\textsuperscript{60-65}. Generally these works have shown that how these dislocation/interface reactions proceed depend on the atomic and defect structure of the interface. Thus, it cannot be readily expected that the nanoscale Mg layers bonded to Nb will behave like nanocrystalline Mg alone or that the semi-coherent HCP Mg/Nb interface would react in a similar manner to an impinging or deposited dislocation as a coherent BCC Mg/Nb interface.

4.1 *Density functional theory calculations*

Deformation mechanisms in nanolayered composites deformation include dislocation slip and interfacial sliding. Thus far, analysis of the 50 nm and 5 nm samples suggest that deformation occurred by plasticity in the layers and not by interfacial slip. While the preferred slip systems in hcp Mg and bcc Nb are known, they are not known in bcc Mg. The favored modes of crystallographic slip strongly depend on the particular electronic and atomic structure
of the material and, hence, those for bcc Mg should be distinct from hcp Mg. It is similar for the ideal shear strengths of the coherent bccMg/bcc Nb and semi-coherent hcpMg/bcc Nb interface. Their differing atomic structures of the interface and adjoining materials would render their interfacial shear strengths different. It may be possible to obtain the interfacial shear strength of the hcp Mg/Nb interface via MD simulations since the interatomic potentials for hcp Mg and bcc Nb exist. However, for the coherent bccMg/bccNb interface, the option for MD calculation is not presently available.

As a way of identifying the preferred slip modes in bcc Mg and propensity for interfacial sliding along the BCC-Nb∥BCC-Mg and BCC-Nb∥HCP-Mg interfaces, we consider calculations of the generalized stacking fault energy curve (GSFE), associated with shearing along these specific crystallographic planes and directions. The GSFE surface is the excess energy per unit area for a given relative displacement vector \( \mathbf{u} \) of one half of the crystal with respect to the other half when a perfect crystal is cut across the slip plane into two parts. In this way, the GSFE provides a calculation of the variation in energy corresponding to the shearing action caused by the glide of a dislocation on specific crystallographic planes. From these calculations, estimates can be attained for the ideal shear stress (ISS) that would resist the shear on a particular mode of slip and the energetically favorable shear displacement paths. The more likely modes on which dislocations would glide in an actual metal would tend to possess the lower values of ISS. In this work, we use first-principles density functional theory (DFT) as implemented in VASP to calculate several possible, geometrically admissible slip modes in bcc Mg.

The DFT calculation and analysis of GSFE curves, however, have a relative character, in the sense that the ease of glide on slip and the interface can be compared by the similar metric and calculation. It does not provide actual CRSS values or even estimates of the Peierls barrier or
friction stress. The ISS from DFT are far from these actual resistances to the shearing action by gliding dislocations (the CRSS) or in the interface (interfacial sliding) in ambient conditions. In fact, CRSS values are typically three to four orders of magnitude lower than the ideal shear stress at 0 K. The relative ratios of the CRSS values among these deformation modes may not be the same as the ratios of the ISS.

In the crystal plasticity (CP) modeling effort to come, the preferred set of slip modes in BCC Mg are needed as this must be given to the model \textit{a priori}. In general, more than one slip mode is used, however some guidance on the ordering of their characteristic strengths would be desired, but is not necessary. These types of information can be provided by the present DFT calculations. Specifically, the DFT analysis can identify the preferred slip families. The CP calculation also needs as input ratios in the critical resolved shear stresses (CRSS) among these modes. This material information is not expected of DFT, but is usually found independently of DFT. The common method is an inverse method, which considers successful fitting of mechanical deformation simulations by CP to several distinct experimental data sets simultaneously (that is, without varying the parameter set from one data set to another on the same material).

In prior work, DFT was used to calculate the GSFE curve for shearing the \{1-10\} and \{1-12\} planes in the \{111\}, \{110\} and \{001\} directions in BCC Mg\textsuperscript{41}. Among these cases, the two systems with the lowest ideal shear stress are the \{1\-\bar{1}\0\} and \{\bar{1}\1\2\} planes in the \{111\}. The peak energies achieved as the planes shift from one stable state to another were nearly the same, respectively at 161.6 mJ/m\textsuperscript{2} and 158.4 mJ/m\textsuperscript{2}. Thus, as in conventionally bcc metals, these two slip systems also are likely in bcc Mg.
In the DFT, we used the generalized gradient approximation (GGA) for the exchange correlation functional with the Perdew-Becke-Erzenhof (PBE) parameterization\textsuperscript{71}. The interaction between valence electrons and ionic cores is treated using PAW potentials. The number of valence electrons in Mg potential that we have taken is 2 and in the Nb potential is 13. We used a plane wave energy cutoff of 400 eV and optimized the structure until the force on each atom is smaller than 0.01 eV/A. We used a 19x19x19 Gamma-centered Monkhorst Pack k-point mesh to integrate the Brillouin Zone of the primitive hcp and bcc unit cells of Mg and Nb to calculate the structural parameters. Table 1 shows calculated lattice constants and elastic constants for the BCC-Nb, HCP-Mg and BCC-Mg from DFT and values are in good agreement with previous calculations and experimental measurements\textsuperscript{72-75}.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>BCC-Nb</th>
<th>HCP-Mg</th>
<th>BCC-Mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>a (Å)</td>
<td>3.307</td>
<td>3.191</td>
<td>3.573</td>
</tr>
<tr>
<td>c/a</td>
<td>1.00</td>
<td>1.623</td>
<td>1.00</td>
</tr>
<tr>
<td>C\textsubscript{11}</td>
<td>253.2</td>
<td>62.7</td>
<td>35.1</td>
</tr>
<tr>
<td>C\textsubscript{33}</td>
<td>66.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C\textsubscript{12}</td>
<td>140.2</td>
<td>27.5</td>
<td>34.7</td>
</tr>
<tr>
<td>C\textsubscript{13}</td>
<td>20.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C\textsubscript{44}</td>
<td>20.3</td>
<td>17.7</td>
<td>29.5</td>
</tr>
<tr>
<td>C\textsubscript{66}</td>
<td></td>
<td>17.6</td>
<td></td>
</tr>
</tbody>
</table>

Table 1: Calculated values for the lattice and elastic constants (in GPa) for the bulk BCC-Nb, HCP-Mg and HCP-Nb obtained from DFT.

For comparison and as a check of the utility of the method, the GSFE curves are obtained for the common slip systems in both single-phase BCC-Mg and single-phase HCP-Mg. We studied the GSFE curves in BCC-Mg for (110) and (112) slip planes, which are most common slip planes in BCC crystals. The periodic model for (110) slip plane contains 48 atoms and its dimensions are 3.57 Å along x, 5.06 Å along y and 75.66 Å along the z. The periodic model for (112) slip plane also contains 48 atoms and its dimensions are 5.06 Å along x, 3.10 Å along y and 85.04 Å along the z. Both supercells contain a thick vacuum layer of 15 Å along the z
direction. The supercell dimensions are chosen based on the minimum number of layers along the z direction for which convergence in system energy is attained. For calculation of the GSFE curves, we used relaxed method\textsuperscript{76}, where we shift the upper half of the crystal with respect to the lower half of the crystal along the glide direction in a small displacement step. Furthermore, at each displacement, we ensured the minimization of the energy of the system by fixing all atomic positions along the glide direction and allowing positions in the z direction and along the direction lying normal to the glide direction to relax. The calculated GSFE curves for slip system in the BCC-Mg are shown in Figure 7(a).

Similarly, we studied the GSFE curves in HCP-Mg for four slip planes: basal, prismatic, pyramidal-I and pyramidal-II. The periodic model for basal slip plane contains 52 atoms and its dimensions are 3.19 Å along x, 5.53 Å along y and 77.17 Å along the z. The periodic model for prismatic slip plane contains 48 atoms and its dimensions are 3.19 Å along x, 5.18 Å along y and 81.33 Å along the z. The periodic model for pyramidal-I slip plane contains 64 atoms and its dimensions are 3.19 Å along x, 11.75 Å along y and 56.49 Å along the z. The periodic model for pyramidal-II slip plane contains 60 atoms and its dimensions are 5.53 Å along x, 6.09 Å along y and 51.49 Å along the z. All these supercells contain a thick vacuum layer of 15 Å along the z direction. The calculated GSFE curves for slip system in the HCP-Mg are shown in Figure 7(b).

To study the GSFE curves for slip at the Mg/Nb coherent interface in DFT, we take supercells consisting of 48 atoms (24 Nb and 24 Mg) as shown in Figure 6(a) and (b). These supercells are periodic along x and y directions. For BCC-Nb||BCC-Mg (cube-on-cube), crystallographic (110) plane of Nb is parallel to (110) plane of Mg, and \{001\} direction in Nb is parallel to \{001\} direction in Mg (Figure 6(a)). For the BCC-Nb||HCP-Mg interface, crystallographic (110) plane of Nb is parallel to (0001) plane of Mg, and \{001\} direction in Nb is
parallel to \(\{1\bar{2}10\}\) direction in Mg (Figure 6(b)). To make two interfaces coherent, we applied equal and opposite strain in the x and y directions for both Nb and Mg layers.

Figure 6 The crystallographic orientation of the bilayer models to study the GSFE curve for slip systems at (a) BCC-Nb\|BCC-Mg interface and (b) BCC-Nb\|HCP-Mg interface.

Figure 7(c) and (d) presents the relaxed normalized GSFE curves for the slip systems at interface for the two interfaces, the bcc Nb/bcc Mg interface and the bcc Nb/hcp Mg interface. From these curves, the ISS can be calculated\(^{67, 77, 78}\). Table 2 shows the calculated ISS values for hcp Mg and bcc Mg. Also, presented for comparison are the ISS values for interface shearing in three in-plane directions of the bcc Nb/bcc Mg interface and the bcc Nb/hcp Mg interface.
Figure 7 Calculated GSFE curves from first-principles DFT method. (a) GSFE for slip systems in the bulk BCC-Mg; (b) GSFE for slip systems in the bulk HCP-Mg; (c) GSFE for slip systems at interface of BCC-Nb||BCC-Mg; (d) GSFE for slip at interface of BCC-Nb||HCP-Mg. The glide directions for the interface plane in (c) and (d) are chosen with respect to crystallographic directions of BCC-Nb in the bilayer systems.
### Table 2

<table>
<thead>
<tr>
<th>Single Phase</th>
<th>Slip Mode</th>
<th>Unstable Stacking Fault (mJ/m²)</th>
<th>[GPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>BCC-Mg</strong></td>
<td>(110)(001)</td>
<td>456.9</td>
<td>3.96</td>
</tr>
<tr>
<td></td>
<td>(110)(110)</td>
<td>454.3</td>
<td>3.27</td>
</tr>
<tr>
<td></td>
<td>(110)(111)</td>
<td>161.0</td>
<td>1.56</td>
</tr>
<tr>
<td></td>
<td>(112)(111)</td>
<td>183.0</td>
<td>1.68</td>
</tr>
<tr>
<td><strong>HCP-Mg</strong></td>
<td>Basal (a)</td>
<td>90.2</td>
<td>1.40</td>
</tr>
<tr>
<td></td>
<td>Prismatic (a)</td>
<td>208.2</td>
<td>2.08</td>
</tr>
<tr>
<td></td>
<td>Pyramidal-I (c + a)</td>
<td>230.0</td>
<td>1.95</td>
</tr>
<tr>
<td></td>
<td>Pyramidal-II (c + a)</td>
<td>257.0</td>
<td>2.16</td>
</tr>
<tr>
<td><strong>Bi-layer</strong></td>
<td>**BCC-Nb</td>
<td></td>
<td>BCC-Mg**</td>
</tr>
<tr>
<td></td>
<td><strong>BCC-Mg</strong> (110)</td>
<td>1127.0</td>
<td>7.84</td>
</tr>
<tr>
<td></td>
<td><strong>BCC-Mg</strong> (111)</td>
<td>505.5</td>
<td>6.07</td>
</tr>
<tr>
<td></td>
<td><strong>HCP-Mg</strong> (001)</td>
<td>347.7</td>
<td>5.27</td>
</tr>
<tr>
<td></td>
<td><strong>HCP-Mg</strong> (110)</td>
<td>973.1</td>
<td>3.35</td>
</tr>
<tr>
<td></td>
<td><strong>HCP-Mg</strong> (111)</td>
<td>303.5</td>
<td>4.75</td>
</tr>
</tbody>
</table>

Comparing BCC Mg to HCP Mg, the ISS for the easiest slip mode basal slip in HCP Mg is lower than that for the easiest slip modes for BCC Mg, {110} and {112}. There is an even smaller difference between the ISS values for {110} and {112} slip in BCC Mg, with the former being slightly easier.

### 4.2 Crystal plasticity finite element modeling method

To help relate particular plastic deformation mechanism to flow responses of nanocomposites containing either HCP Mg or BCC Mg, a model of the Mg/Nb nanolayered composites using crystal plasticity finite element (CPFE) framework was built. The same CPFE models for the normal and parallel cases are applied.
Figure 8 shows a meshed granular bilayer of Mg and Nb for the 50-50 nm sample and 5-5 nm sample. Both models are divided into two equal sections/volumes that represent a particular layer of Mg and Nb, in which one grain spans through the layer thickness. Two separate FE grain microstructure meshes were generated, in which grains have different aspect ratios.

![Figure 8](image)

**Figure 8** The CPFE model meshes for (a) the 50 – 50 nm Mg/Nb composite and (b) the 5-5 nm composite. Each model contains one layer each of Mg and Nb. Bottom images show zoomed-in view of the microstructures indicating different grain aspect ratio.

The initial microstructure was set as close as possible to that of the PVD samples. In the 50-50 nm model, grains are nearly equiaxed with grain 50 nm thick and 100 nm wide. In the 5-5 nm model, their thickness is reduced from 50 nm to 5 nm, while in the plane of the layers they retain the same size and shape, i.e., the grains have pancake like shape. Grain orientations were randomly selected from the initial measured texture (Fig. 1). For the 50-50 nm model, grains in the Mg phase and the Nb phase were assigned orientations randomly selected from their corresponding measured textures taken from the as-fabricated 50-50 nm composite. For the 5-5 nm model, the Mg and Nb phases had the same texture. Mg and Nb grain pairs joined by their mutual interface plane (011) were given the same orientation, producing a cube-on-cube
orientation relationship. For the 50-50 nm, Mg and Nb grain pairs shared a common \{0001\}||\{011\} interface plane.

In both FE models, granular microstructure is made to be periodic. The FE meshes consist of roughly 1 million and 435,000 C3D4 (continuum three-dimensional four-nodal) elements, in the 50-50 nm and 5-5 nm cases respectively. In both models each layer consists of exactly 267 grains (total 534 grains in both layers).

The model is used to simulate simple compression. We use periodic boundary conditions, wherein the deformation of each pair of boundary faces (top/bottom, front/back and left/right) is equal and as a result the stress tensors on each pair are opposite in sign. The simple compression boundary conditions are prescribed by specifying the displacement along the loading direction (negative z-direction – normal case (loading axis is normal to the layers), negative x-direction – parallel case (loading axis is parallel to the layers)), while the lateral faces were kept free to expand.

The constitutive law used at every integration point accounts for both elastic anisotropy and plasticity by crystallographic slip. The formulation for the used in CPFE is given in many prior works\(^77,79-81\). 

\textit{Elasticity.} For the 50 – 50 nm composite, the elastic constants for the Mg and Nb phases were assigned their bulk values, which are for HCP Mg: \(C_{11} = 59.5\) GPa, \(C_{12} = 26.1\) GPa, \(C_{13} = 21.8\) GPa, \(C_{33} = 65.6\) GPa, \(C_{44} = 16.3\) GPa\(^75\) and for BCC Nb: \(C_{11} = 267\) GPa, \(C_{12} = 134\) GPa, \(C_{44} = 28.7\) GPa\(^82\). For the 5-5 nm, elastic modulus measurements of 5 nm Mg and 5 nm Nb in this composite do not exist to our knowledge. Since our interest lies in the active deformation mechanisms during plastic deformation, we made a reasonable guess for the elastic response of this nanolayered composite. First the bcc Nb phase is presumed to possess the same
elastic properties as bulk Nb. Second, we assumed the bcc Mg phase exhibited cubic elastic anisotropy, which includes three independent elastic constants. Next, we fit the elastic portion of the composite response to compression tests made normal, parallel and 45 degrees from the interface plane (Figures 9 and 10). This approach produces an estimate for the elastic constants of $C_{11} = 65$ GPa, $C_{12} = 35$ GPa, $C_{44} = 22.5$ GPa.

Figure 9 Comparison between the measured true stress-true strain hcpMg/bccNb micropillar compression responses and simulated elastic responses for 50-50 nm composites for (a) normal, (b) parallel and (c) 45° deformation cases.
Figure 10 Comparison between the measured true stress-true strain bccMg/bccNb micropillar compression responses and simulated elastic responses for 5-5 nm composites for (a) normal, (b) parallel and (c) 45° deformation cases.

Plasticity. For the crystal plasticity part of the constitutive law, it is necessary to specify the slip and twin families on which slip is expected to occur. The plastic deformation of hcp Mg occurs by slip and twinning. The three main slip modes made available in the model are for hcp Mg are basal (a) slip, prismatic (a) slip, and pyramidal (c + a) \{1122\}(1123) slip. In the present case, deformation twinning was not detected via post mortem TEM analysis and as mentioned the stress-strain curves did not exhibit the usual signs of twinning. Thus, it is likely that twinning...
occurs infrequently or not at all. Although, twinning could be taken into account in the modeling as it has been in prior work\textsuperscript{32, 87}, it is removed in the present study as interests lie in the difference in slip properties of hcp vs bcc Mg. In order to model bcc Nb, the two slip modes made available are \{110\}\{111\} slip and \{112\}\{111\} slip. Based on the DFT results, these two slip modes are also made available to bcc Mg.

The last significant part of the constitutive law is the model for the critical resolved shear stress (CRSS), the characteristic stress that needs to be overcome in order for the dislocation to glide. The resistance to glide on individual slip modes \(\alpha\) has many contributions: geometric hardening due to the texture, a friction stress \(\tau_0^{\alpha}\), which is independent of interactions with other dislocations and the interfaces, and another component, which is dependent on them \(\tau_{\text{disl}}^{\alpha}(h^{\alpha})\), giving the following:

\[
\tau_c^{\alpha} = \tau_0^{\alpha} + \tau_{\text{disl}}^{\alpha}(h^{\alpha}).
\]

The latter resistance \(\tau_{\text{disl}}^{\alpha}(h^{\alpha})\) depends on how dislocations move and accumulate in the layers. In the present case, the interfaces are spaced sufficiently close, < 50 nm, which is only one order of magnitude from the dislocation core. Thus the movement of dislocations could be treated individually as well as the local interactions of dislocations with the interface. Also, dislocations do not accumulate in the layers to the level that they can be considered as a homogeneous density, making it less accurate to not consider how they glide or their proximity to the nearly by interfaces.

The interfaces confine the movement of the dislocations, forcing them to thread through the layers, depositing in the interfaces as they pass by\textsuperscript{52-55}. This picture of dislocation motion is adopted in the confined layer slip model (CLS). A threading dislocation can experience a resistance to slip \(\tau_{\text{CLS}}^{\alpha}\) that increases as the layer thickness \(h\) decreases\textsuperscript{52, 53}. The increasing
difficulty to glide as size $h$ reduces provides a direct size effect to slip resistance. Derivation of $\tau_{CLS}^{\alpha}$ is based on continuum dislocation theory and applies at the nanoscale inside an individual layer, where a single dislocation moves. In the conventional application of the CLS law, the CLS size effect is usually directly translated to explain the size effect in the strength or hardness of the nanolayered composite\textsuperscript{52-55}.

In this work, however, a multiscale model is developed to relate the effects of $h$ on dislocation glide resistance to the flow stress-strain response of the composite. At the lowest length scale treated by the model, the total CRSS value is given as a resistance to slip, a threshold value needed in the flow rule that relates the slip rate on a slip system to the resolved shear stress on that system. CP theory is then used to relate the activity of slip (the slip rates in a crystal) to the distortion of that crystal. The same theory is used in all crystals, but the distortion of each crystal is different depending on its orientation with respect to the loading and its own particular history of deformation.

Some distinctions between the analytical CLS model and the present computational CP model are worth noting. As one difference from the analytical model, the discrete computational model here makes the link between CLS at the smallest scale to the macroscopic behavior at the largest scale. The size scaling in macroscopic strength with $h$ will not necessarily follow the same size scaling in CRSS at the nanoscale. Second, as another difference, in the analytical model, a single slip system operates in the layer. However, the crystals in the CP model will generally deform by more than one slip system and even by more than one slip mode, such as in an HCP or BCC material. Therefore, as many slip systems as needed to deform the crystal are allowed to operate in the same crystal.

In this work, a generalized form of the CLS is given by:
\[ \tau_{\text{disl}}^{\alpha}(h^s, \alpha, s) = \tau_{\text{CLS}}^{\alpha}(h^{s'}) = A^\alpha \frac{\mu^\alpha b^\alpha}{h^{s'}} \ln \left( \frac{c h^{s'}}{b^\alpha} \right) + \frac{f^\alpha b^\alpha}{h^{s'}}, \]

where \( h^{s'} \) is the minimum distance along the slip plane of slip system \( s \) spanned between adjacent interfaces. Thus, \( h^{s'} \) depends on the orientation of the crystal with respect to the interface normal and the layer thickness \( h \). Hereinafter we drop the superscript \( \alpha \) and \( s \) on variables \( h', A \), and \( f \).

The original CLS model of 52 is still largely intact in eqn (3) and minor modifications are made, such as the removal of the Taylor factor \( M \) and the logarithmic energy pre-factor dependent on screw/edge character. We also have made parameters \( \tau_0^\alpha \), \( A \), and \( f \) dependent on slip family \( \alpha \), and the particular interface and dislocation that are interacting. The core cut-off parameter \( c \) ranges from unity to \( \sqrt{2} \) and is set to unity in the calculations below. Analogous with the previous works that have applied the CLS model to multilayers, the expected order of magnitude for \( \tau_0^\alpha \) is 10-100 MPa, for \( A \) is \( 10^{-2} \) to \( 10^{-1} \), and for \( fb \) is 1 to 3 J/m\(^2\).

The first term \( \tau_0^\alpha \) depends on the slip family and does not change as the microstructure evolves with strain. It represents the sum of a friction stress and resistance from other obstacles, which would not significantly altered by strain. The second term, which bears an \( \ln(h)/h \) dependence, results from the resistance encountered by the dislocation as it propagates through the layer. \( A \) is related to the self-energy of the dislocation deposited in the interface and would depend on dislocation and interface type. It can evolve through its dependence on \( h' \). The last term, i.e., \( fb/h \), results from the deformation of the interface caused by the threading dislocation. It represents the change in energy of the interface caused by the interaction with the threading dislocation loop as it moves through the layer. The displacement shift \( D \) in the interface caused by the dislocation alters locally the interface energy \( \sigma = (d\gamma/dD) \). If we let \( \gamma \) be the interface
energy in units of energy per unit area of interface \([\text{mJ/m}^2]\) and normalize \(D\) with respect to the shear strain \(\varepsilon\) caused by the moving dislocation \(b/h'\) then the final term is \(\sigma = d\gamma/dn\ (b/h')\). Thus \(\sigma\) can be re-expressed as the product of \(f = d\gamma/dn\), which depends on the interface and dislocation interacting and geometry, \(b/h'\). This resistive interface stress, when positive, means the shear strain caused by the dislocation resists the motion of the dislocation. Like the second term, this last contribution can also evolve during the deformation simulation, since both texture and layer thickness \(h\) can change with strain, causing \(h'\), to change.

In the modeling, \(\tau_0^{\alpha}\), \(A\), and \(f\) are used as fitting parameters, where the first depends on material and dislocation family and the last two depend additionally on interface. In the calculations that follow, we assume that all slip systems belonging to a given slip mode \(\alpha\) have the same CRSS, but these could differ from one slip mode to another. Since \(\tau_0^{\alpha}\) is considered a material parameter, the same value was given to the Nb phase in all composites, in both the 5 nm and 50 nm. Hence, differences in \(\tau_0^{\alpha}\), due to changes in lattice parameter in Nb was neglected. Based on the DFT results for ISS, the same value of \(\tau_0^{\alpha}\) was assigned for the \{110\} and \{112\} slip modes. Similarly for BCC Mg, \(\tau_0^{\alpha}\) was the same for \{110\} and \{112\} slip, but was different than those of BCC Nb. For HCP Mg, \(\tau_0^{\alpha}\) varied between the basal, prismatic, and pyramidal \(\langle c + a \rangle\) slip modes. The order and values for \(\tau_0^{\alpha}\) were not taken from DFT and they were used instead as fitting parameters.
(a) 50-50 nm

<table>
<thead>
<tr>
<th>α - Slip mode</th>
<th>basal slip</th>
<th>prismatic slip</th>
<th>pyramidal slip</th>
<th>{110} and {112}</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_{0,f}$ [MPa]</td>
<td>40</td>
<td>70</td>
<td>240</td>
<td>495</td>
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</tbody>
</table>

(b) 50-50 nm

<table>
<thead>
<tr>
<th>α - Slip mode</th>
<th>basal slip</th>
<th>prismatic slip</th>
<th>pyramidal slip</th>
<th>{110} and {112}</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A^\alpha$</td>
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<td>0.4</td>
<td>0.3</td>
<td>0.35</td>
</tr>
<tr>
<td>$f^\alpha$</td>
<td>8.65</td>
<td>11.64</td>
<td>12.27</td>
<td>24.2</td>
</tr>
<tr>
<td>$b^\alpha [x10^{-10} m]$</td>
<td>3.2094</td>
<td>3.2094</td>
<td>6.1197</td>
<td>2.8579</td>
</tr>
<tr>
<td>$\mu^\alpha [GPa]$</td>
<td>16.5</td>
<td>16.5</td>
<td>16.5</td>
<td>28.7</td>
</tr>
</tbody>
</table>

(c) 5-5 nm

<table>
<thead>
<tr>
<th>α - Slip mode</th>
<th>Mg {110} and {112}</th>
<th>Nb {110} and {112}</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_{0,f}^\alpha$ [MPa]</td>
<td>185</td>
<td>495</td>
</tr>
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</table>

(d) 5-5 nm

<table>
<thead>
<tr>
<th>α - Slip mode</th>
<th>Mg {110} and {112}</th>
<th>Nb {110} and {112}</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A^\alpha$</td>
<td>0.067</td>
<td>0.157</td>
</tr>
<tr>
<td>$f^\alpha$</td>
<td>3.19</td>
<td>4.13</td>
</tr>
<tr>
<td>$b^\alpha [x10^{-10} m]$</td>
<td>3.347</td>
<td>3.347</td>
</tr>
<tr>
<td>$\mu^\alpha [GPa]$</td>
<td>22.5</td>
<td>28.7</td>
</tr>
</tbody>
</table>

Table 3. Material parameters used in CLS model.

5. Results

The CP model is applied to simulate the elastic-plastic deformation of the 5 nm and 50 nm Mg/Nb composites from the beginning of loading to the peak stress. Figure 11 compares the calculated stress-strain curves using the parameter set in Table 3 and the experimental measurements for the normal and parallel loading cases. As shown, in each test, the agreement is reasonable in yield stress and hardening rate. The plastic anisotropy in compression, in which the normal loading is higher than the parallel loading, is also captured. In particular, for the $h = 50$ nm case, the degree of anisotropy agrees well with the experiment, but it is underestimated for
the $h = 5$ nm composite. Last, as in the measurement, the model flow stresses for the bcc Mg composite in both loading directions, are higher than that of the hcp Mg composite.

The values of the parameters in Table 3 can be considered part of the output of the model. Overall, their values are in a physically permissible range and consistent with those expected from prior CLS studies$^{52-55}$. The values for $\tau_0^{\alpha}$ are material properties, independent of orientation. It is found that $\tau_0^{\alpha}$ for pyramidal $\langle c + a \rangle$ slip is higher than prismatic $\langle a \rangle$ slip, which are both higher than that for basal $\langle a \rangle$ slip. This ordering of slip mode resistances is consistent with the ISS calculated from DFT, as well as many prior CP studies on bulk HCP Mg alloy studies$^{38, 39, 49}$. $A$ pertains to the local change in the core of the dislocation when deposited in the interface and $f$ to the response of the interface to the local deformation caused by the deposited dislocation. It is found from the analysis here that generally, $A$ and $f$, for the HCP and BCC slip modes are lower for the coherent BCC/BCC interface than HCP/BCC interface. This difference prevails for all values of $A$ and $f$ regardless of the type of dislocation. However, because the dislocations in the HCP Mg are not the same as those in the BCC Mg, analysis of interface effects on slip resistance are better evaluated by comparing the $\{112\}$ and $\{110\}$ dislocations in the Nb phase of the two composites. The smaller $A$ would imply that the dislocation core has a lower self-energy in the coherent interface than in the semi-coherent one. The smaller, and positive, value for $f$ for the coherent interface implies that this interface resists the shift caused by the dislocation, less so than the semi-coherent one.

The same model predicts as output the slip activities in each crystal at each strain level. Figures FIFTY-SLIP and FIVE-SLIP present, respectively for the $h = 50$ nm and 5 nm composite, the bulk average contributions of slip rate for each slip mode to the deformation of its phase, either Mg or Nb. In this way, the proportional of the strain accommodated by each phase
and each mode in each phase can be assessed. In all simulations, the model presumes that slip is confined to the layers, and with this assumption, uncovers the type of slip activated during each test. For the normal loading cases, the applied strain for the first 2% is entirely accommodated by deformation of the Mg phase. In the 50 nm composite, basal slip dominates Mg phase deformation particularly, initially. As straining proceeds, basal slip activity decreases, while prismatic and pyramidal activity increases, such that all three operate in similar amounts at the strain at which the peak stress is reached. In the Nb phase in this composite, \{112\} slip is more active than \{110\} slip and remains so during deformation. The calculations for the 5 nm composite, find that the Nb behaves similarly as it does in the 50 nm composite. In the 5 nm BCC Mg phase, both slip modes are active, but as in the Nb phase, the \{112\} slip mode dominates.

The model is used to determine the source of the macroscopic hardening rate. Typically in a bulk material, macroscopic hardening arises due to storage of dislocations. In the present case, however, there is no evidence of dislocation storage from TEM, and dislocation storage was not taken into account in the model. The CRSS law used was not dependent on the instantaneous dislocation density stored, but instead depended on \(h\) and the orientation of the crystal via \(h'\). The interpretation of the model is that the hardening seen in Figures 11 is due to a combination of a reduction in \(h\) and change in texture. The hardening is thus higher in the normal case than parallel case, since in the normal case, the reduction in \(h\) during deformation is more severe.

Next, the model is used to seek an explanation for the anisotropy seen between the normal and parallel test cases for the same \(h\) value. From Table 3, it is evident that Nb is the stronger material compared to Mg, whether Mg is HCP or BCC. From Figures 12 and 13, in both composites, it is observed that Nb accommodates proportionally more applied strain in normal
loading than parallel loading, which would alone cause normal loading to give rise to a higher flow stress. This would explain the anisotropy seen in both the \( h = 50 \text{ nm} \) and \( 5 \text{ nm} \) composites. For the \( h = 50 \text{ nm} \) HCP Mg composite, the difference is additionally due to more \( \langle c + a \rangle \) slip activity in the Mg phase in normal loading than parallel. According to Table 3, \( \langle c + a \rangle \) slip had the highest value for \( \tau_0^\alpha \) than those for prismatic and basal slip. Thus, activity of the hardest mode in normal loading but not in parallel would contribute to the higher flow stress.

Finally, using the model results, the origin of the higher strength of bcc Mg composite for the hcp Mg composite is examined. This comparison is not straightforward, since admittedly these two composites differ in a few highly influential aspects that can govern strength: size and interface type. For aid, the model parameters in Table 3 are analyzed, first those independent of size, such as \( \tau_0^\alpha \), and second those dependent on size, such as \( h \) and indirectly, the interface type, \( A \) and \( f \). In Nb, the \( \tau_0^\alpha \) values for the two slip modes are the same for the two composites. The texture and slip activities between the two modes are similar as well. Thus, the deformation behavior of the Nb phase cannot explain the higher flow stress of the \( 5 \text{ nm} \) composite. However, for Mg, \( \tau_0^\alpha \) values are higher for the \( \{110\} \) and \( \{112\} \) slip systems in the BCC Mg than \( \tau_0^\alpha \) for basal and prismatic slip, the two more active slip systems in HCP Mg in both normal and parallel loading. Thus, it is suggested that BCC Mg possesses a higher intrinsic glide resistance than HCP Mg, leading to strengthening. Second, the BCC Mg composite has a much finer layer thickness, \( h = 5 \text{ nm} \) vs \( 50 \text{ nm} \), and this alone can provide substantial strengthening, an effect that has been directly incorporated into the size independent CLS law in eqn (1). Nonetheless, it is worth examining the effect of interface type itself. As mentioned earlier, for all dislocation types, \( A \) and \( f \) are smaller for coherent BCC/BCC interface than the semi-coherent HCP/BCC interface, indicating that the coherent BCC/BCC provides less resistance to CLS than the semi-coherent
HCP/BCC. Hence, putting the value of $h$ aside, the implication is that the interface resistance in a composite with the coherent interface is less than that in a composite with the semi-coherent HCP/BCC. To summarize, analysis of the model predictions and associated parameters suggests that the higher strength from the BCC composite is due to two factors, the increase in resistance to threading primarily due to the finer layer thickness and increase in $\tau_0^\alpha$ of the BCC Mg slip modes compared to those of the two easiest HCP Mg slip modes.

![Graphs](image.png)

**Figure 11** Comparison of the predicted and measured stress-strain curves from micropillar compression for the (a) 50-50 nm Mg/Nb composites and (b) 5-5 nm BCCMg/Nb composites.
Figure 12 Calculated slip activity for the 5-5 nm BCC Mg/Nb composites.
6. Discussion

The model calculations have assumed that both Mg and Nb phases of both composites deformed by slip and the interface remains intact during deformation. Furthermore, slip is confined to the layers and does not transmit across the layers via slip transmission. Therefore, the implicit assumption made here is that the stress to transmit slip across the layers, $\tau_{\text{trans}}$, is presumed higher than that to glide in the layers. Since the layer thicknesses $h$, representing the critical length-scale affecting dislocation motion, lie in the range of $h = 5$ to $50$ nm, slip is considered to operate by threading through the layers and presumed to experience an $h$-dependent resistance to threading, according to the CLS model, eqn (1). The resistance increases as $\ln(h)/h$ and thus it is possible that at the finer layer thickness studied here, i.e., $h = 5$ nm, threading through the layers could become difficult, too high that the stress for slip to transmit $\tau_{\text{trans}}$ across interfaces is less and thus more favorable. The value for $\tau_{\text{trans}}$ for the coherent BCC Mg/Nb has not been calculated. For reference, we mention calculations of $\tau_{\text{trans}}$ for a single dislocation to transmit slip across a coherent Cu/Ni interface. The $\tau_{\text{trans}}$ stress lies in the regime of 0.3 GPa to 1 GPa according to MD calculations and meso-scale calculations$^{88-91}$. For

Figure 13 Calculated slip activity for the 5-5 nm BCC Mg/Nb composites.
In MD simulations of Cu/Nb nanolaminates, involving nucleation and glide of multiple dislocations, found that initially dislocations emit from interfaces and grain boundaries and thread through the layers and only later in deformation does slip transmission occur. Last, hardness measurements of the BCC Mg/Nb composites show a consistent strengthening with reduction in \( h \) from 50 nm to 5 nm (see Figure 3). One sign that slip transmission prevails would be a critical \( h \) below which hardness does not continue to increase and for the present composites this value may be 5 nm or smaller. Thus, while no evidence exists to suggest that slip transmission dominates, it cannot be ruled out entirely, particularly in the case of the \( h = 5 \) nm BCC Mg/Nb composite and especially with increased straining. To our knowledge this work is the first attempt to incorporate the CLS model into CPFE and to include both slip transmission and CLS would lie beyond the scope of this work. Only a few CP models to date, in fact, have attempted to incorporate slip transmission into their models.

A comprehensive assessment of hardness and strength measurements of several nanotwinned and two-phase multilayer systems was recently carried out. Notably for all systems, all strength metrics, and over a broad nanoscale range of \( h \) from 100 nm to 10 nm, “smaller proved stronger”, and size-dependent strengthening followed a two-parameter, Hall-Petch scaling law. One interesting outcome was the significant gap in strength between the homophase nanotwinned materials and the bi-phase materials for the same layer thickness. Model interpretation of the CLS law in this work could provide an explanation based on differences in interface type; the energetic parameters \( A \) and \( f \) were consistently lower for the coherent interface than the semi-coherent one. On this basis, it may be that the coherent interface in the
nanotwinned materials provided less resistance to dislocation propagation than the two-phase semi-coherent one.

One of the useful predictions of the model is slip activity. In the HCP Mg phase, the slip activity shows that basal slip prevails, a result which is not surprising for pure Mg, and is consistent with many reports of pure Mg in many coarse and ultra-fine Mg based systems. The model indicates that \{112\} slip dominates the slip activity over \{110\} slip in the Nb phase in both composites and in the BCC Mg phase in both loading directions. Both the \{112\} and \{110\} slip modes had the same friction stress. Thus, the higher propensity for \{112\} slip is a consequence of geometry. Two factors affecting activation can be related to geometry. The first is texture, or the current orientation of the crystal with respect to the load, which affects the resolved shear stress (RSS), which is compared to the critical resolved shear stress. The second is the projected layer thickness \(h'\), which depends on both the current orientation of the crystal and current layer thickness. It affects the CRSS via eqn (2).

To isolate the two geometric-based sources affecting slip activity, we removed the CLS hardening by setting \(A = 0\) in eqn (2). The results find that \{112\} slip is still favored over \{110\} slip, indicating that the texture is likely responsible for the predominance of \{112\} slip. The distribution of orientations with respect to the loading states must result in higher local RSS values on the \{112\} slip systems than the \{110\} slip systems in the grains. To confirm this, we carried a few more simulations without CLS hardening. First, we changed both initial texture, considering a classical rolled BCC texture, and the applied loading state to plane strain compression, an ideal representation of the deformation during rolling. Changing the initial texture to a rolled texture, the \{112\} slip was more active than \{110\} slip during uniaxial simple compression. However, slip in \{110\} slip was more active than \{112\} slip when changing to
plane strain compression loading while keeping the initial texture as measured. Thus, slip activity on the \{112\} slip systems is more active than \{110\} slip is primarily a consequence of the initial texture with respect to the simple compression loading both normal and parallel during micropillar compression.

It is interesting to find a few aspects of deformation that were not affected by layer size h. First is the slip activity. As mentioned, the dominance of \{112\} slip is due to texture effects and for the Nb phase and BCC Mg phase, the texture did not change as the layer thickness reduced. The second aspect is the proportion of the load carried by Mg vs Nb. In both the h = 5 nm and 50 nm composite, the Mg phase initially in the first few percent of strain, accommodated the applied deformation. Last, is the deformation behavior of the Nb phase. The slip activity and proportion of load carried by the Nb phase changed only when the direction of loading changed and not as the layer thickness, interface type, and Mg phase changed between the two composites. Many of these similarities can be explained simply by considering that the main deformation mode remained slip in the layers as opposed to interfacial deformation, and that the Nb phase did not change and remained the stronger phase as the Mg changed phase from HCP to BCC. These findings need to be supported by repeating studies with different h but for the same composite type, whether HCP Mg/Nb or BCCMg/Nb.

7. Conclusions

In this work, a combination of experiment and computational techniques were used to gain insight into the deformation mechanisms underlying the room temperature deformation of the bcc Mg phase in nanolayered composites. Both multilayered 5/5 nm bcc Mg/bcc Nb (5 nm bccMg) and 50/50 nm hcp Mg/bcc Nb (50 nm hcpMg) composites are fabricated via physical vapor deposition and tested via micropilar compression. The 5 nm bccMg composite exhibited
50% higher strength and larger strains to failure when compressed normal and parallel to the layers than the 50 nm hcpMg composites. Post-mortem TEM analysis of the deformed pillars suggests co-deformation and no twinning during compression normal to the interfaces. To interpret these results, we carry out DFT calculations of generalized stacking fault energy curves and crystal plasticity based calculations of pillar compression using a crystal plasticity finite element model. DFT indicates that in bcc Mg, glide \{110\}(111) and \{112\}(111) slip systems would be easier than other glide systems and also shearing in the bccMg/bccNb interface. A crystal plasticity finite element model is built to simulate the compression deformation of the pillar. It adopted an experimental grain structure and texture and a constitutive law that took into account elastic deformation and inelastic deformation by crystal plasticity. The model newly introduces confined layer slip for dislocation glide resistance at the slip system level in place of the conventional layer size-independent dislocation density hardening law. They also indicate that the stress-strain response of the 5 nm bccMg composite results from dislocation mediated plasticity in both the bcc Mg phase and Nb phase on the \{110\}(111) and \{112\}(111) slip systems. The 5 nm bccMg is stronger than the 50 nm hcpMg one due to the reduction in layer thickness and that glide on the \{110\}(111) and \{112\}(111) slip systems is relatively harder than basal slip in hcp Mg.

**Acknowledgements**

M. A., M. J., S.P., and M.K. acknowledge funding from the National Science Foundation (NSF) - Civil, Mechanical and Manufacturing Innovation (CMMI) Early Concept Grants for Exploratory Research (EAGER) grant #1541918. S.P. gratefully acknowledges support from the University of Nevada, Reno Research Enhancement Grant 2017 for this work. A. K. would like to acknowledge LANL LDRD program #20170680ER for financial support. I. J. B.
acknowledges financial support from the National Science Foundation (NSF CMMI-1728224).

We acknowledge support from the Center for Scientific Computing from the CNSI, MRL: an NSF MRSEC (DMR-1121053). Part of the research was performed at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy 97 Office of Science. Los Alamos National Laboratory is operated by Los Alamos National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under Contract No. DE-AC52-06NA25396.

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Chapter 6

This chapter was published as: Explicit incorporation of deformation twins into crystal plasticity finite element models, Milan Ardeljan, Rodney J. McCabe, Irene J. Beyerlein, Marko Knezevic, Computer Methods in Applied Mechanics and Engineering, 295, 396-413. My role in preparing this chapter was to develop a novel procedure for explicit modeling of discrete twin lamellae within crystal plasticity finite element framework. I successfully applied the developed model to study twinning behavior in uranium. I performed the modeling work presented in this chapter and also processed all the data to create the necessary figures that led to important conclusions. Furthermore, I prepared the first draft of the paper and I was actively contributing in the process of producing the final draft along with my co-authors.
Explicit incorporation of deformation twins into crystal plasticity finite element models

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Abstract

Deformation twinning is a subgrain mechanism that strongly influences the mechanical response and microstructural evolution of metals especially those with low symmetry crystal structure. In this work, we present an approach to modeling the morphological and crystallographic reorientation associated with the formation and thickening of a twin lamella within a crystal plasticity finite element (CPFE) framework. The CPFE model is modified for the first time to include the shear transformation strain associated with deformation twinning. Using this model, we study the stress-strain fields and relative activities of the active deformation modes before and after the formation of a twin and during thickening within the twin, and in the parent grain close to the twin and away from the twin boundaries. These calculations are carried out in cast uranium (U), which has an orthorhombic crystal structure and twins predominantly on the \{130\} \langle3\bar{1}0\rangle systems under ambient conditions. The results show that the resolved shear stresses on a given twin system on the twin–parent grain interface and in the parent are highly inhomogeneous. We use the calculated mechanical fields to determine whether the twin evolution occurs via thickening of the existing twin lamella or formation of a second twin lamella. The analysis suggests that the driving force for thickening the existing twin lamella is low and that formation of multiple twin lamellae is energetically more favorable. The overall modeling framework and insight into why twins in U tend to be thin are described and discussed in this paper.
Keywords: Crystal plasticity finite element models; Stress fields; Deformation twinning; Twin formation; Twin thickening

1. Introduction

Deformation twinning plays a significant role in the deformation response of many metals and their alloys, particularly those with low symmetry crystal structures, such as hexagonal close packed Mg, Zr, Be, Ti and orthorhombic uranium (U). To accommodate a general deformation state, these polycrystalline metals activate both dislocation slip and twinning \[1-9\]. The relative resistance and contributions of these two modes can evolve differently with strain and strain direction \[4, 10-12\]. As a result, these metals exhibit a highly anisotropic mechanical response. Understanding the interplay of slip and twinning at the microscopic level and its influence on the macroscopic response are premier challenges in constitutive modeling of low symmetry materials. Additionally, there are fundamental questions regarding how and where twinning initiates, why a single lamella would thicken in one case while multiple lamellae would form in another, and when twinning saturates.

In the past, many studies have used materials models to link polycrystalline flow stress and hardening to slip and twinning within the individual crystals. Reproducing the effects of deformation twinning is usually more demanding and challenging than for slip. Deformation twins affect the microstructure in two ways: they reorient the lattice in a finite domain within a grain, and they introduce a twin-matrix boundary between the original parent grain and the twin domain \[3, 13\]. Current models incorporating twins include analytical models \[14\], polycrystalline mean-field schemes such as Taylor \[15-23\] and self-consistent models \[24, 25\], and spatially resolved techniques, such as crystal plasticity finite element (CPFE) \[26-34\] and Green’s function fast Fourier transform (FFT) \[35, 36\] models. Typically, polycrystalline mean-
field models account for the shear produced by twinning by modeling it as a pseudo-slip process \cite{37, 38}. At the same time, they consider the reorientation effect in one of several ways, either via: (i) the predominant twin reorientation (PTR) method \cite{38}, (ii) the volume fraction transfer (VFT) scheme \cite{12}, (iii) the total Lagrangian approach \cite{17, 30}, or (iv) the composite grain (CG) method \cite{11}. While successful in capturing the macroscopic stress-strain response and bulk texture evolution \cite{39, 40}, these schemes do not capture the dynamic and spatially heterogeneous nature of twinning. A particularly important limitation is their inability to account for the resolved shear stress at the twin–parent grain interface responsible for thickening of an existing twin.

Spatial full-field techniques can explicitly incorporate the characteristic twin shear and corresponding grain reorientation and, therefore, better capture fields associated with subsequent twin thickening. To understand the local stress distribution as a consequence of twin formation, phenomenological finite element modeling has been utilized to model a twin in Zr \cite{41, 42}. A cuboidal inclusion representing a parent grain that develops a twin was embedded in an isotropic medium. As such, the effects of morphology and local grain structure on the fields were not taken into account. Moreover plastic anisotropy of the inclusion was accounted for using a macroscopic Hill’s yield criterion \cite{43}. The study correlated the stress states that are energetically favorable for twinning with twin volume fraction and morphology. More recently, a full-field, elasto-viscoplastic formulation based on the Green’s function FFT method was used to study distributions of local stress states around a twin in Mg \cite{36}. The study revealed the variation in the shear stress profile on the twin planes consistent with the lenticular shape of twins. However, modeling of twin thickening and the associated evolution of the mechanical fields have not been modeled using the FFT technique.
Explicit incorporation of deformation twinning in CPFE has not been attempted thus far. With CPFE, a polycrystal is discretized into finite elements and a crystal plasticity constitutive law operates at each FE integration point. Both stress equilibrium and strain compatibility are satisfied providing better predictions of local and overall material behavior and microstructure evolution. In CPFE, one of the main difficulties is related to FE mesh manipulation. Remeshing of every grain containing one twin or multiple twins must be performed at the initial twin formation stage and every step during twin thickening. These mesh alterations computationally intensify the already intensive calculations involved in CPFE codes.

The main objective of this work is to develop a numerical procedure for explicit 3D modeling of the formation and thickening of twin lamellae under imposed plastic deformation conditions into the CPFE framework. The novel procedure explicitly models twin transformation, i.e., the characteristic twin shear and crystallographic reorientation of the twinned domains. Moreover, the effect of both the twin transformation shear and neighboring grain shape in 3D on the local stress distribution are modeled. In addition to twin formation and thickening, the model captures grain-to-grain interactions and their effect on the mechanical fields. To showcase this capability, we apply the newly developed twin-CPFE model to study twinning in U. Specifically, we treat the case of twin lamellae formation and thickening within a grain in U favorably oriented for twinning, which is surrounded by other grains that are not favorably oriented for twinning. The analysis aims to demonstrate how the technique can provide unique insights into the changes in the stress state and in slip mode activity in the parent and twin grain after the initial twin formation and during twin thickening. As an example, two scenarios for twin expansion are considered: expansion of the first lamella formed or formation of a second lamella and no further expansion of the first lamella. We use resolved shear stress fields and
strain energy density arguments to indicate which scenario would be more favorable. For the particular material and microstructure considered here, the latter is favored. The technique developed here is intended as a simulation tool to study the development of deformation twins within a microstructural and mechanical framework.

The paper is structured as follows. In section 2, the modelling framework, including the kinematics and hardening models, is presented. In section 3, the selected material, uranium, for the study is discussed. In section 4, we present the methodology and computational tools developed to model the formation and thickening of a twin lamella. In section 5, we show and discuss the results of a case study on twin growth in uranium. In section 6, we finalize the article with a few concluding remarks.

2. Modeling framework

A modeling framework is presented here using a notation that is now standard in continuum mechanics. We denote tensors using boldface symbols and not italicized ones, while scalars are italicized and not boldfaced. In this notation, \( \mathbf{F} \) represents the deformation gradient tensor, \( \mathbf{L} \) represents the velocity gradient tensor, and \( \mathbf{\sigma} \) represents the Cauchy stress tensor. In this framework, the formulation described below is enforced at each integration point within each element in the finite mesh to relate the stress to the strain work conjugate.

2.1. Kinematics of slip and twinning within CPFE

The applied velocity gradient tensor, \( \mathbf{L} \), is given by

\[
\mathbf{L} = \mathbf{L}^e + \mathbf{L}^p
\]  

where \( \mathbf{L}^e \) and \( \mathbf{L}^p \) are the elastic and plastic velocity gradients, respectively. The plastic velocity gradient contains the contributions from slip and twinning via

\[
\mathbf{L}^p = \mathbf{L}^{sl} + \mathbf{L}^{tw}.
\]  

The expressions for the velocity gradients, due to slip and twinning, are respectively:
\[
L_{sl} = \sum_{\alpha}^{N_{sl}} \dot{\gamma}_\alpha \mathbf{m}_\alpha^0,
\]
\[
L_{tw} = \sum_{\beta}^{N_{tw}} \dot{f}_\beta S^\beta \mathbf{m}_\beta^0,
\]
\[\text{(3)}\]
where \(\dot{\gamma}_\alpha\) is the shearing rate on the slip system \(\alpha\), \(\mathbf{m}_\alpha^0\) and \(\mathbf{m}_\beta^\beta\) are Schmid tensors of the slip system \(\alpha\) and twin system \(\beta\), respectively, \(S^\beta\) is the characteristic twin shear, and \(N_{sl}\) and \(N_{tw}\) are the total number of available slip and twin systems, respectively. The Schmid tensors are the unit slip (or twin) system tensor, defined as the dyadic product of two orthogonal unit vectors denoting the slip (or twin) shear direction and the slip (or twin) plane normal, respectively. The subscript ‘o’ in the total Lagrangian framework employed in this work indicates that these tensors are defined using the initial crystal orientation and therefore the tensors are known \textit{a priori}.

The rate of change of the twin volume fraction per twin system, \(\dot{f}^\beta\), is based on the pseudo slip model \([30, 38]\), given by \(\dot{f}^\beta = \frac{\dot{\gamma}^\beta}{S^\beta}\), or in a given strain increment by \(\Delta f^\beta = \frac{\Delta \gamma^\beta}{S^\beta}\). If in \(n\) strain increments, the volume fraction of a particular twin system, \(\beta\), reaches unity, i.e., \(\sum_1^n \Delta f^\beta = 1\), then
\[
S^\beta = \sum_1^n \Delta \gamma^\beta.
\]
\[\text{(4)}\]
The pseudo slip model accounts for twinning shear strains in the same manner as it does for slip. It only considers the shear accommodated by twinning, but does not account for the reorientation or the formation of a twin domain.

For finite deformations, the total deformation gradient tensor \(\mathbf{F}\) can be decomposed into elastic and plastic components as:
\[
\mathbf{F} = \mathbf{F}^e \mathbf{F}^p,
\]
\[\text{(5)}\]
where \(\mathbf{F}^e\) contains deformation gradients due to both elastic stretching and lattice rotation, while \(\mathbf{F}^p\) denotes the deformation gradient because of plastic deformation alone. The evolution of \(\mathbf{F}^p\) can be expressed in a rate form using the following flow rule relationship:
\[
\dot{F}^p = L^p F^p. 
\]

After integration from \( t \) to \( \tau = t + \Delta t \), Eq. (6) becomes:

\[
F^p(\tau) = \exp(L^p \Delta t) F^p(t). 
\]

We can further approximate the exponential as:

\[
F^p(\tau) = (I + \Delta t L^p) F^p(t) = (I + \Delta t (L^{sl} + L^{tw})) F^p(t), 
\]

where \( I \) is the identity matrix. The constitutive equation for stress in the crystal is expressed as:

\[
T^e = CE^e, \quad T^e = F^{-1} ((\text{det} F^e) \sigma) F^{-T}, \quad E^e = \frac{1}{2} \{ F^e T^e F^e - I \}, 
\]

where \( C \) is the fourth-order elasticity tensor, \( T^e \) is the second Piola-Kirchhoff stress, which is elastic work conjugate to the Lagrangian finite strain \( E^e \), and \( \sigma \) is the Cauchy stress in the crystal. To calculate stress, we need to evaluate \( F^e = FF^{-1} \). Therefore we can rewrite Eq. (8) as:

\[
F^{-1}(\tau) = F^{-1}(t) \{ I - \Delta t (L^{sl} + L^{tw}) \}. 
\]

Next, we divide \( L^{tw} \) into two parts, \( L^{tw,pts} \) and \( L^{tw,ots} \), i.e.,

\[
L^{tw} = L^{tw,pts} + L^{tw,ots}. 
\]

In Eq. (11), \( L^{tw,pts} \) is the velocity gradient of the most active variant, which we will call the predominant twin system (pts) and \( L^{tw,ots} \) is the velocity gradient from all other twin systems (ots) contributing to plasticity.

### 2.2 Kinetics of the slip and twinning mechanism

In order to estimate the shear strain rate, \( \dot{\gamma}^\alpha \), for each slip system \( \alpha \), and the shear strain rate, \( \dot{\gamma}^\beta \), for each twinning system \( \beta \), we can relate the resolved shear stress (\( \tau^\alpha = T^e \cdot m_0^\alpha \) for slip and \( \tau^\beta = T^e \cdot m_0^\beta \) for twinning) on the system to the characteristic resistance \( \tau_c^\alpha \) for slip systems and \( \tau_c^\beta \) for twin systems according to the following power-law relationships [30, 44, 45]:

244
\[
\dot{\gamma}^\alpha = \dot{\gamma}_0 \left( \frac{|\tau_{c?\alpha}|}{\tau_{c?\alpha}} \right)^{\frac{1}{m}} \text{sign}(\tau^\alpha), \quad \dot{\gamma}^\beta = \begin{cases} 
\dot{\gamma}_0 \left( \frac{|\tau_{c?\beta}|}{\tau_{c?\beta}} \right)^{\frac{1}{m}} \text{sign}(\tau^\beta) & \text{if } \tau^\beta > 0 \\
0 & \text{if } \tau^\beta < 0 
\end{cases}
\]

(12)

where \(\dot{\gamma}_0\) is a reference slip rate (arbitrarily taken here as 0.001 s\(^{-1}\)) and \(m\) represents the strain rate sensitivity factor (taken here to be 0.02 for both slip and twinning systems).

2.3 **Hardening laws for slip and twinning**

In this work, we use a dislocation density hardening law formulation to compute the evolution of the slip and twin resistances as a function of strain, temperature, and strain rate [40, 46]. It is assumed that all slip and twin systems within the same deformation mode share the same values for critical resolved shear stress (CRSS). This hardening law has been successfully used to model deformation of several metals within mean-field self-consistent codes, differing in crystal structure, such as Haynes 25 [47], AA6022 [48], Nb [49, 50], Ta [51, 52], Mg [53-55], Zr [46, 56, 57], Be [10, 58], and U [4, 59, 60]. Here, we integrate the same hardening law for U in CPFE and enable the existing CPFE to model the orthorhombic structure. Below is a brief review of this model.

The critical resolved shear stress for activation of slip considers contributions of several different terms: a friction stress \(\tau_{0,f}^\alpha\), a forest dislocation interaction stress \(\tau_{for}^\alpha\) and a dislocation substructure interaction stress \(\tau_{sub}^\alpha\):

\[
\tau_{c?}^\alpha = \tau_{0,f}^\alpha + \tau_{for}^\alpha + \tau_{sub}^\alpha.
\]

(13)

The model for the critical resolved shear stress for twin activation is distinct from that for slip. It accounts for a temperature-independent friction term \(\tau_{0}^\beta\) and a latent hardening term coupling the active slip and the twin systems. Taken together, the critical resolved shear stress for twinning can be expressed as:

\[
\tau_{c?}^\beta = \tau_{0}^\beta + \mu^\beta \sum_\alpha C^{\alpha\beta} b^\beta b^\alpha \rho_{for}^\alpha.
\]

(14)
Here $\mu^\beta$, $b^\beta$ and $C^\alpha\beta$ represent the elastic shear modulus, Burgers vector on the given twin system, and the latent hardening matrix used for coupling of slip and twin systems, respectively.

The behavior of $\tau_{for}^\alpha$ and $\tau_{sub}^\alpha$ is governed by the evolution of the dislocation densities in the form of forest $\rho_{for}^\alpha$ and substructure $\rho_{sub}^\alpha$ dislocations. These relationships, for each dislocation type, can be expressed in the form of a Taylor law:

$$\tau_{for}^\alpha = \chi b^\alpha \mu^\alpha \sqrt{\rho_{for}^\alpha}, \text{ and}$$

$$\tau_{sub}^\alpha = k_{sub} b^\alpha \mu^\alpha \sqrt{\log \left( \frac{1}{b^\alpha \sqrt{\rho_{sub}}} \right)}$$

where $\chi = 0.9$ is a dislocation interaction parameter, $\mu^\alpha$ is the shear modulus and $k_{sub} = 0.086$ is a mathematical parameter that insures that Eq. (15) recovers the Taylor law at low dislocation densities [61]. Equation (16) is related to substructure stress required for gliding dislocations to bow out and punch through arrays of locked dislocation segments that are closely spaced at later stages of hardening [61]. The stored forest density $\rho_{for}^\alpha$ evolves via a competition between the rate of storage and the rate of dynamic recovery:

$$\frac{\partial \rho_{for}^\alpha}{\partial \gamma^\alpha} = \frac{\partial \rho_{gen,for}^\alpha}{\partial \gamma^\alpha} - \frac{\partial \rho_{rem,for}^\alpha}{\partial \gamma^\alpha} = k_1^\alpha \sqrt{\rho_{for}^\alpha} - k_2^\alpha (\dot{\varepsilon}, T) \rho_{for}^\alpha,$$

$$\Delta \rho_{for}^\alpha = \frac{\partial \rho_{for}^\alpha}{\partial \gamma^\alpha} \left| \Delta \gamma^\alpha \right|$$

where $k_1^\alpha$ is a coefficient for the rate of dislocation storage due to statistical trapping of gliding dislocations by the forest obstacles and $k_2^\alpha$ is the coefficient for the rate of dynamic recovery, which is given by the following expression: [46]

$$\frac{k_2^\alpha (\dot{\varepsilon}, T)}{k_1^\alpha} = \frac{\chi b^\alpha}{g^\alpha} \left( 1 - \frac{kT}{D^\alpha b^\alpha} \ln \left( \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \right) \right).$$

In Eq. (19), $k$, $\dot{\varepsilon}_0$, $g^\alpha$ and $D^\alpha$ are respectively Boltzmann’s constant, a reference strain rate, an effective activation enthalpy and a drag stress. The drag stress for dislocation apply to dislocation speeds within the thermally activated regime where phonon effects can be reasonably
neglected [62]. It has been proposed and suggested via discrete dislocation dynamics simulations that the processes accountable for dynamic recovery are similar to those that lead to the formation of dislocation substructures, patterns of dislocations, such as cell walls and dislocation sheets. Dislocation interactions can result in the formation of jogs, dipoles, and lock that self-organize under deformation into relatively low energy-structures [63]. In our model, the increment in substructure development is proportional to the rate of dynamic recovery of all active dislocations and can be expressed as:

$$\Delta \rho_{sub} = \sum_\alpha q b^\alpha \frac{\partial \rho_{rem,for}^\alpha}{\partial \gamma^\alpha} |\Delta \gamma^\alpha|, \quad (20)$$

where $q$ is a coefficient defining the fraction of an $\alpha$-type dislocations that do not annihilate but become substructure dislocation. The hardening parameters have been calibrated in the earlier study [59] and will be used here.

3. Deformation mechanisms of uranium

Under the ambient conditions modeled here, U has a base-centered orthorhombic crystal structure, where the unit cell dimensions are $a = 0.2852$, $b = 0.5865$ and $c = 0.4945$ nm. Because of the low crystallographic symmetry, U deforms by both slip and twinning mechanisms [8, 9, 64, 65]. The most dominant slip modes observed in U are $(010)[100]$ and $(001)[100]$, with only one independent slip system in each. The two other slip modes found active in U are $\frac{1}{2}\{110\}(1\overline{1}0)$ and $\frac{1}{2}\{021\}(1\overline{1}2)$, with two and four slip systems, respectively. The prominent deformation twin in U is $\{130\}(3\overline{1}0)$, and the value of its characteristic twin shear is 0.299. The $\{172\}(3\overline{1}2)$ twin mode, and its reciprocal twin $\{112\}(3\overline{7}2)$ mode both with characteristic shears of 0.227, have also been observed. The characteristic twinning shear values are based on crystallography and are taken from [3, 8, 9]. The, $\{130\}(3\overline{1}0)$ and $\{172\}(3\overline{1}2)$ twin modes
reorient the crystal lattice by 69.3° about [001] and 92.6° about <1070>, respectively. Specific geometries of the U slip and twin systems are shown in Fig. 1. Figure 2 shows orientation maps based on the electron backscattered diffraction (EBSD) of a deformed microstructure of cast U at a strain of 0.05. In slight contrast to the typical EBSD image of deformed Mg alloys [5], Zr [57], or Ti [39], we observe a large number of relatively thin twin lamellae per grain in cast U. The origin of this unusual twin morphology has yet to be understood.

<table>
<thead>
<tr>
<th></th>
<th>(010)[001]</th>
<th>(001)[100]</th>
<th>1/2{110}(110)</th>
<th>1/2{021}(112)</th>
<th>{130}(310)</th>
<th>{172}(312)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Slip System</td>
<td>1 Slip System</td>
<td>2 Slip Systems</td>
<td>4 Slip Systems</td>
<td>2 Twin Variants</td>
<td>4 Twin Variants</td>
<td></td>
</tr>
</tbody>
</table>

**Figure 1** Slip and twin systems in uranium. The arrow shows the Burgers vector direction in the plane.

**Figure 2** EBSD-based scan of tension direction orientation map of the microstructure for the cast uranium studied here. The colors in the orientation map represent the orientation of the ND sample direction with respect to the grain orientations.
4. Explicit incorporation of twinning in CPFE

The flow chart in Fig. 3 illustrates the overall procedure for twin formation and thickening within CPFE. This procedure is explained next.

Create voxel-based polycrystalline microstructures

Define finite element mesh of grain structure

Perform deformation (simple compression)

Extract surface mesh of individual grains

**Twin formation**

Select grains developing $f_{tw,pts}$

Define twin planes corresponding to $\beta_{tw,pts}$

Intersect grain surface mesh with twin planes

Generate surface mesh over parent grain and twin

**Twin thickening**

Select grains with growing $f_{tw,pts}$

Define twin planes corresponding to $\beta_{tw,pts}$

Intersect grain surface mesh with twin planes

Generate surface mesh over parent grain and twin
Figure 3 Modeling framework for explicit incorporation of twinning in CPFE.

4.1 Finite element model of the grain structure

A synthetic microstructure is generated first in the publicly available software DREAM.3D [66, 67]. We find that DREAM.3D generates grains that are more realistic in terms of grain morphology and grain size distribution than those typically generated using the Voronoi tessellation scheme. It overcomes several limitations of Voronoi tessellation. Generally, the Voronoi tessellation begins with random seeds, which produces a near-equiaxed set of domains (or grains). It is possible to place seeds far apart in one dimension to get elongated grains, but it is difficult to control the aspect ratios. Also, with Voronoi tessellations it is difficult to obtain size or shape distributions that have "heavy tails". The distributions of these parameters tend to be fairly normally distributed by the nature of the process. Furthermore, because the boundary between the two domains/grains is placed halfway between the seed points, it is challenging to obtain grain neighbors of disparate sizes, i.e., large grains next to small grains. Lastly, Voronoi tessellations yield perfectly planar boundaries, which may be significantly different from those of real grain boundaries.

DREAM.3D generates 3D synthetic voxel-based microstructure and surface meshes for each individual grain based on a specified grain size and grain shape distributions. Furthermore, we define voxel density/resolution in the model in order to achieve the desired number of surface
finite elements. A surface mesh is the bridge between a voxel-based model and a volumetric (in our case tetrahedral) mesh, and is the foundation for successful 3D mesh generation. Starting from the surface mesh, we perform 3D solid meshing of individual grains ensuring mesh conformance between grain boundaries using Patran [68]. We refer to this as ‘conformal’ grain boundaries, an aspect that is critical to modeling grain-to-grain interactions and is not found in other spatially resolved, full-field techniques such as the Green’s function FFT method [35]. The reader can find a detailed step-by-step explanation of this meshing procedure in [28]. Figure 3a shows the final voxel-based and meshed microstructures used in the present study. In order to unveil the interior of the model and to show the grain morphologies, we cut the model in half and expose two cut planes (see the two right-most images in Fig. 4).

**Figure 4** A finite element model of an explicit grain structure consisting of 27 grains and 480000 C3D4 elements. The two sections on the right show the internal grain structure. The red grain in the center has a crystallographic orientation selected to favor \{130\} <310> twinning.

The FE model of the 3D microstructure contains 27 grains and approximately 480000 finite elements (each grain consists of approximately 18000 finite elements). As shown, these large U grains are packed in a cube with an edge length of 1.0 mm. In order to discretize the whole volume, we use linear tetrahedral elements each with one integration point (type C3D4 in ABAQUS). In our previous study [28], we performed a detailed analysis regarding the selection of the elements type and size. From there, we observed that the use of higher-order elements (e.g.
C3D10M) does not significantly affect the distribution of stress-strain fields or the prediction of texture and grain boundaries. Because these microstructures consist of grains with highly irregular shapes, meshing with a very large number of linear finite elements, which are computationally less intensive, overcomes the benefits of meshing with a smaller number of higher order elements, which are computationally more intensive.

We arbitrarily assign crystal orientations that would not develop substantial twin activity to every grain except the red grain in the center of the FE model. The crystal orientation of this grain is selected such that it favors the twinning system (130)[310] under simple compression along the normal direction, ND (the axis Z in Fig. 4). The particular orientation defined by Bunge-Euler angles is (0°, 90°, 10°). Crystal orientations of other grains do not develop twins during the early stage of simple compression deformation. The same crystal orientation is assigned to each finite element within a corresponding grain, which results in the initial intra-granular misorientations of zero for each grain.

The simple compression is performed by imposing displacement in the Z direction (or the normal direction, ND) with the lateral sides traction-free and, hence, free to expand (Fig. 3a). The compression consists of several deformation steps, necessary to initially form and then thicken the twin lamella. It was interrupted at three different strain levels corresponding to (1) 1% of a twin variant volume fraction, (2) 3% volume fraction thickening of the twin lamella, and (3) 5% volume fraction thickening of the twin lamella. When the twin volume fraction of the predominant twin system (pts) reaches a threshold value of 1% of the central grain’s volume an initial twin lamella is formed. Next, we describe the model for twin formation and thickening.
4.2 Procedure for incorporating twin lamellae in an FE mesh

Explicitly including a twin lamella into the finite element framework requires development of an automated procedure. The procedure is detailed in the flowchart in Fig. 3 and as shown, consists of several geometric manipulations and mesh generations. We have developed a script in Matlab [69], which writes Patran and Python script files containing specific commands for Patran and Abaqus, respectively. The Patran scripts are executed within Patran to perform either surface or solid meshing and the Python script files are executed within Abaqus to either extract the surface mesh from the solid mesh model or to perform the Abaqus mesh cleanup procedure [70]. The final result of this procedure is a twin lamella of a desired volume inserted in a selected parent grain that maintains the overall conformity with the parent and neighboring grains.

After a deformation step, the procedure starts by obtaining the surface mesh of the deformed grains. This step applies regardless of whether a new twin lamella is first formed or a pre-existing twin lamella thickens for a prescribed volume increment. Extraction of the surface mesh is achieved using a Python script written by the Matlab script containing the appropriate commands for Abaqus. The output of this Python script is surface meshes of all deformed grains. At this point the procedure continues with either forming or thickening a twin lamella. This step is shown in the Fig. 3b and c of the flow chart. The Matlab script finds the intersection points between the two cutting planes (that form a twin) and the 3D surface mesh of the parent grain and prepares a Patran script. The Patran script uses coordinates of these points for each intersected plane and connects them into a single closed loop or "chain" consisting of line segments. The script contains the commands to generate and export surface meshes for each intersection plane. It is important to mention that these newly generated triangular elements are of the same size as the ones that build the surface of the intersected grain. The control is then
returned to the Matlab script. To preserve the mesh conformity of the grain boundaries of neighboring grains touching the twin, the surface meshes of these neighboring grains are also adjusted (Fig. 3d). At this point, we assemble the model that is made of individual grain surface meshes. This model has only grain boundaries that are conformal. Next, the Matlab script writes a Python script for surface mesh cleanup in Abaqus to collapse any elements with bad aspect ratio. The mesh repair procedure collapses elements with the edge aspect ratio greater than 4. Note that the mesh repair procedure is not performed on individual grain surface meshes because that would ruin the overall mesh conformity between grains when assembling them over the surface mesh of the entire model. The Patran script is then generated and called upon to perform 3D meshing for each individual grain and twin. This step starts from the surface meshes to ensure the overall conformity of the mesh. Finally, the Matlab script writes an Abaqus input file containing the new mesh, state variables, and boundary conditions for the subsequent deformation step.

In carrying out the above procedure, careful attempts are made to minimize changes made to the model microstructure. After meshing, the following state variables: \( \mathbf{F} \), dislocation densities and crystal orientations (preserving any developed intra-grain misorientation), are mapped onto the new mesh. For this mapping, we used a scheme to find the closest elements from the “old” mesh (before forming or growing the twin) to the “newly” created elements (after meshing) and assigning the state variables from the old mesh to the new mesh based on the mutual proximity of the element centroids. In that sense, the overall deformation state of the model and crystal orientations are transferred and preserved from the “old” to the “new” mesh.

The frequency of remeshing procedures is important in order to capture the changes that occur in the stress-strain fields in the material due to twin formation and thickening, which are
relevant to twin evolution. In the case of uranium, twin thickening of 2\% volume fraction was
determined to be sufficient to reveal the fields. Due to the very fine mesh within every grain in
the model, remapping of the state variables from the “old” mesh to the “new” mesh is performed
with success, which will be later shown in the evolution of the stress fields in the parent and twin
grain at different values of twin volume fraction.

This entire procedure is repeated on every occasion when we want to form new twin lamellae
or to grow pre-existing twin lamellae.

4.2.1 Twin lamella formation

After the volume fraction of the \( \beta = tw,pts \) in a grain reaches a pre-specified threshold value,
we insert a twin lamella. In the present study, the threshold value of 1\% is chosen. The volume
fraction of the \( \beta = tw,pts \) is calculated as the integral of the \( \beta = tw,pts \) volume fraction over every
element set representing a grain (after convergence is achieved in each strain increment). When
the threshold is reached, the deformation is interrupted in order to insert the lamella. Note that
the evolution of twin volume fraction is calculated within the CPFE model at the end of every
strain increment and checked whether the threshold is reached.

The geometry of the created lamella is uniquely determined by the twin plane normal of the
\( \beta = tw,pts \) twin variant and the thickness of the lamella, which is calculated to produce a
specified total twin volume fraction, which in this work is 1\%. The twin planes span the entire
grain.

4.2.2 Location of twin lamella formation

To create the twin lamella, an important question concerns where to place it within the parent
grain. Twins are thought to originate from grain boundaries at points of highest stress
concentration [71]. To determine the location of the highest stress concentration on the surface of
the parent grain, we use the von Mises stress normalized by the average value calculated over the entire volume of the model. Figure 5a shows the contours over the grain, Fig. 5b the actual location where the initial twin lamella has been placed, and Fig. 5 c-f the orientation relationship between the stress concentrations and the location of the twin lamella. In this example, the highest stress concentration lies at the grain boundary where the parent grain meets three other neighboring grains, (i.e., a quadruple point). Starting from this point, we form a twin lamella by inserting two parallel planes across the parent grain with a specified separation to match the twin volume fraction. The planes have a normal vector corresponding to the twin plane of the $\mathit{pts}$ and the twin shear is imposed within this plane in the direction of the Burgers vector of the twin.

Figure 5 Distributions of the von Mises stress ($\overline{\text{VMises}}$) normalized by the applied stress over the parent grain (a) without a twin lamella, (b) after the formation of 1\% twin lamella, (c-d) Y-Z sections (c) before and (d) after 1\% twin formation, and (e-f) X-Z sections (e) before and (f) after 1\% twin formation.
4.2.3 Characteristic twin shear accommodation by the twin lamella

Thus far, we have discussed one important aspect of the model, which is the ability to introduce a discrete twin lamella within a grain with a twin volume fraction based on the total twinning activity accumulated within the grain. For this we described the needed geometric and FE mesh manipulations. To fully model the twin, we must also consider the other aspect of twinning, which is its transformation into a reoriented volume with a characteristic twin shear. To this end, we describe how we account for both the reorientation and shearing action imposed by the created twin lamella. Specifically, the kinematics and kinetics related to the twin shear strain and the behavior of the parent grain immediately before and after are discussed.

In the freshly formed twin as well as during subsequent twin thickening, $F_p(\tau)$ in the twin is enforced to be:

$$F_p^{-1}(\tau) = \{I - S^{tw,pts}m_0^{tw,pts}\}. \tag{21}$$

Next, the deformation within the parent grain needs to be updated. A twin that is forming and growing within a grain contributes to accommodating the strain applied to the grain. Consequently, the plastic deformation in the parent grain will change according to:

$$F_p^{-1}(\tau) = F_p^{-1}(t)\{I + f^{tw,pts}S^{tw,pts}m_0^{tw,pts}\}, \tag{22}$$

where $f^{tw,pts}$ is the accumulated volume fraction of the twin. The superscript denotes the variant $\beta = tw,pts$ that has been selected. Eqns. 21 and 22 together represent the transfer of strain after a twin has formed. Eq. 21 ensures that the strain accommodated by this variant is transferred to the twin and produces the appropriate thickness, while Eq. 22 ensures that it is removed from the parent grain. For numerical stability, the update of $F_p$ in the parent grain and twin at each FE integration point is carried out using a specified number of much smaller strain
(or time) increments than that used to simulate the increment in the applied simple compression deformation. The updated values of $F^p$ for all elements within the parent grain and twin are enforced simultaneously during this ‘intermediate period’ and while the entire grain structure model is held under the applied simple compression strain.

4.3 Twin thickening

As we apply more strain to the model, a twin is permitted to expand in prescribed increments from the initial 1% twin volume fraction. For demonstration, we consider thickening the initial twin to volume fractions of 3% and 5%. For this, the FE mesh is altered in a similar manner as twin formation. Maintaining the same twin normal and location of the initially formed twin, we cut the surface mesh of the parent grain by two parallel planes with a specified separation in order to expand the twin volume (Fig. 3). In this case, the surface mesh of the parent grain is now reduced for the volume of the previously formed twin lamella. The distance between the cutting planes is changed in order to reflect the twin growth. Also, the characteristic shear strain of the twin is enforced using Eqs. (19 and 20). Expansion is performed on both sides of the twin until the prescribed twin volume is achieved. For the sake of simplicity, the same twin normal used for twin formation is maintained during twin growth. It is important to emphasize, however, that in our numerical framework, the twin boundary could take on a different normal during growth. Figures 6 and 7 show the parent grain and the grain cluster model after the twin lamella is first created and after it grows to 3% twin volume fraction.
Figure 6 (a) FE mesh of the grain favorably oriented for twinning. (b) Parent and twin grain after creating the twin lamella of 1% volume fraction. (c) Parent grain and twin after twin growth from 1% to 3% volume fraction. Note the small change in shape of the grain under deformation. The original FE mesh of the parent grain has not changed substantially after the twin lamella is introduced except in close proximity to the twin lamella.

Figure 7 Twin formation and thickening with respect to the surrounding neighboring grains in the 3D model: (a) initial grain structure, (b) grain structure with 1% formed twin and (c) grain structure with 3% twin.

5. Application: a case study of twinning in uranium

Having described the CPFE-twinning model, we now, in this section, apply it to simulate the initial formation and thickening of twin lamellae during mechanical loading. We consider simple compression of the U grain structure shown in Fig. 4. The crystal orientation of the central (red) grain was chosen to be favorably oriented for twinning, whereas those of the surrounding grains were chosen to be unfavorably oriented. This arrangement allows us to demonstrate twin modeling in the central (parent) grain only, and to analyze the stress fields in the twin, parent
grain, and non-twinning neighbors. We will also discuss the evolution of slip activity within the parent grain before and after twinning and in the twin lamellae as it evolves.

The incremental deformation steps were 0.05 compressive true strain up to the point where 1% twin volume fraction accumulates. At this stage, the 1% volume fraction twin lamella was created (Section 4.2). As described earlier (Section 4.2.2), the twin location is determined by points of high von Mises stress concentration in the boundary. Afterwards, the incremental deformation steps increased to 0.07 compressive true strain to the point where an additional 2% twin volume fraction accumulates (according to the pseudo-slip model for twinning). At this point, we expand the original twin from 1% to 3% volume fraction (Section 4.3).

Figure 5 compares the normalized Von Mises stress distributions during deformation before twinning and as a function of twin volume fraction after twinning. The stress distributions are heterogeneous, reflecting the effect of interactions between neighboring grains differing in crystallography. In particular, high stress concentrations are seen to develop in the neighboring grains in the vicinity where the twin lamella intersects the grain boundary. These are localized areas where the neighboring grain is accommodating the twin shear produced by the twin lamella.

To identify the areas of high probability of twin formation and thickening, in Fig. 8 we show the contour plots of resolved shear stresses on the most dominant twinning plane and in the twin direction (denoted as RSSTW) as a function of twin volume fraction. These resolved shear stresses are normalized by the current value of twin resistance. As expected, large RSSTW values develop in the center grain, confirming that it is oriented well for twinning, while the relatively low RSSTW values in the neighboring grains show that they are not. After forming the 1% twin, the driving force for twin propagation decreases in the regions where the twin-matrix
interface intersects the grain boundary. This reduction can be seen by the drop in RSSTW below 1.0. Therefore, additional straining must be applied such that the RSSTW reaches 1.0 in these areas. After a true strain increment of 0.07 is applied, twinning activity accumulates corresponding to twin growth from 1% to 3%. Figs. 9a and b show the resolved shear stress on the interface just before expansion to 3% volume fraction. After twin thickening to 3%, the RSSTW decreases suggesting that continued twin expansion might be hindered. At the same time, the RSSTW value inside the twin is zero or negative (Fig. 9c). However, away from the twin-matrix interface and within the matrix region, the driving force is high (RSSTW = 1) suggesting that nucleation of another lamella may be favored over continued thickening of the 3% twin. In other words, if the stress were maintained or increased, accommodating more strain via an increase in twin volume fraction is more likely to occur by nucleating a second twin lamella than by expanding the original twin lamella.

Figure 8 Distributions of normalized resolved shear stresses (RSSTW) along the most dominant twin plane in the twin direction for different twin volume percentage (a) no twin, (b) 1% twin, and (c) 3% twin. Note that neighboring grains do not exhibit the propensity for twinning.
Before transformation | After transformation | After continuous deformation

(a) $b_{tw,pts}$

(b)

(c) $\bar{RSSTW}$

(d)

**Figure 9** Distributions of normalized resolved shear stress ($\bar{RSSTW}$) along (a) the left interfacial planes between matrix and the twin lamella, (b) the right interfacial planes between matrix and the twin lamella, (c) a plane in the middle of the twin, and (d) slightly away in the matrix region from the right interface where the second twin lamella has formed. Different stages of deformation are shown as indicated in the figure.

To investigate the likelihood of thickening the first twin lamella versus formation of a second twin lamella, we create one model for thickening the existing twin lamella and another model for forming a separate but parallel twin lamella of the same twin variant while not thickening the
existing twin lamella. A strain increment of 0.06 strain was sufficient to accumulate the twin volume fractions from 3% to 5%. Figure 10 shows the two models, which both produce a total of 5% twin volume fraction. One model consists of growing the 3% twin to a 5% twin and the other model contains the original 3% twin and a second separate 2% twin. The second twin was placed in a region where the stress concentrations in the grain boundaries were high. Figure 11 shows the normalized von Mises contours. As before, stress concentrations at the tips of the twin lamellae within neighboring grains are evident. The RSSTW contours are shown in Fig. 12.

**Figure 10** Grain structures with a parent grain containing (a) one 5% twin lamella and (b) two lamellae one of 2% and another of 3% volume fraction.

**Figure 11** Distributions of normalized value of equivalent stresses ($\bar{\text{VMises}}$) for 5% twin volume fraction for one lamella twin and two twin lamellae.
Figure 12 Distributions of normalized resolved shear stresses (RSSTW) along the most dominant twin plane in the twin direction for different 5% twin volume fraction (a) one lamella and (b) two lamellae.

In order to assess which scenario is more likely to occur, we first consider changes in plastic work $\Delta W_s$ associated with the transformation from a 3% twin lamella to the new twin state, $s$, which is generically given by:

$$\Delta W_s = \frac{1}{V} \sum_1^n \int_V \sigma_{ij} \varepsilon_{ij}^p$$

(23)

where $V$ is the domain of integration. The two work terms of interest are $\Delta W_1$, associated with growth to a single twin lamella at 5% and the other $\Delta W_2$, associated with the state consisting of two lamellae, the original that remains at 3% and a new one at 2%. We can further consider the difference in these two work terms, i.e.,

$$\Delta W = \Delta W_1 - \Delta W_2.$$  

(24)

In calculating $\Delta W_1$ and $\Delta W_2$, the increments in plastic strain $\varepsilon_{ij}^p$, go from 1 to $n$ and we consider the states $s$ after the same amount of applied deformation. We repeat calculation of these work terms for three domains $V$ for the integration: the whole grain cluster, only the parent
and twin lamellae combined, and the parent grain and twin lamellae separately. The results are listed in Table I. As shown, the value of $\Delta W$ for all three domain types suggest that forming a secondary twin lamella with 2% volume fraction is more energetically favorable than increasing the volume fraction of the original one by 2%.

**Table I** Comparison of plastic work calculated over the volume indicated in the table with one lamella vs. two twin lamellae.

<table>
<thead>
<tr>
<th>Work integral (Eqns. 23 and 24)</th>
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<th>$\Delta W_2$ $\left[ \frac{MJ}{m^3} \right] \times 10^4$</th>
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<tbody>
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<td>Grain cluster</td>
<td>5.15</td>
<td>2.30</td>
<td>2.30</td>
</tr>
<tr>
<td>Parent grain + twin</td>
<td>2.30</td>
<td>1.24</td>
<td>1.06</td>
</tr>
<tr>
<td>Parent grain</td>
<td>1.49</td>
<td>0.74</td>
<td>0.75</td>
</tr>
<tr>
<td>Twin lamella</td>
<td>0.81</td>
<td>0.50</td>
<td>0.31</td>
</tr>
</tbody>
</table>

The foregoing application considers just one of many questions relevant to twin growth. There are many possible scenarios of twin growth, such as nucleation of many fine twins, subsequent transmission into the neighboring grains, merging of neighboring twins, etc. The likelihood of each event would depend on the local stress fields imposed by the twins, parent, and neighboring grains while under deformation. Thus, testing for these possibilities calls for a technique such as the one developed here that can simultaneously treat the formation and expansion of discrete twin lamellae in a polycrystal calculation and provide spatially resolved mechanical fields. For demonstration, we considered the possibility of two twin configurations yielding the same twin volume fraction of 5%. Comparing the energy densities indicates that that generation of secondary twin lamella is more likely to occur. This prediction is consistent with experimental observations that a large number of fine twin lamellae often form within U grains (See Fig. 2). However, we should note that this is not expected to apply in general. Other effects
such as parent grain morphology, other grain-neighborhoods, and the number, location and placement of other twin lamellae in 3D space are important factors impacting twin growth. A systematic study of these factors is possible with this technique, but beyond the scope of the present work.

Last, we apply the model to study the accompanying changes in slip activity due to the presence of the discrete twin lamellae. In U, there are four slip modes that can be activated within the parent grain and twin lamellae. Formation of a twin within a grain can affect the choice of slip modes with in the twin. To elucidate any possible changes, we present in Fig. 13 the contours of the most active slip modes. The plots reflect the accumulated value of relative activities for all four slip modes “incrementally”. By this, we mean that at the end of each deformation step for each finite element we identify the slip mode with the highest slip activity within that increment. From the contour plots a change in the predominant slip mode from the $\{021\}\overline{112}$ mode to the $(010)[100]$ mode within the parent grain can be seen when the twin first forms. As the twin lamella expands or a second twin lamella forms, the $(010)[100]$ mode remains predominant in the parent. Within the twin lamellae, the prevalent modes are $\{110\}\overline{110}$ and $(001)[100]$. Interestingly, at the twin-matrix interface there is a shift between the most active slip modes, suggesting a possible loss of the twin-matrix orientation relationship with deformation, which is yet another reason for hampering the existing twin lamella from thickening. By comparing Figs. 13d and e, we can see that the slip activity within the parent and twin lamellae does not change whether one or two lamellae form.
Figure 13 Distributions of the most active slip modes at (a) no twin, (b) 1% twin, (c) 3% twin, (d) 5% one lamella twin and (e) 5% two lamellae twin. Slip mode IDs: 1. (010)[100], 2. $\frac{1}{2}\{110\}(1\overline{1}0)$, 3. (001)[100], 4. $\frac{1}{2}\{021\}(1\overline{1}2)$.

In closing we mention that while the study presented here has focused on fundamental understanding of changes in stress-strain fields due to twin formation and thickening, extending the framework to calculations of many grains that twin is left for future work. The developed procedure is fully automated; however, to facilitate calculations involving thousands of grains, significant increases in computation speed are necessary. To this end, we plan to explore the use of non-iterative numerical methods that are based on fast Fourier transforms [20, 33, 72-77] and utilization of specialized computer hardware [18, 78] that involves graphic hardware.

6. Conclusions

In this paper, we present a novel approach for modelling deformation twinning by explicit incorporation of twin lamellae into a 3D crystal plasticity finite element framework. The
framework is applied to uranium, a material with an orthorhombic crystal structure. Effects of the microstructural characteristics such as grain structure and grain boundaries are explicitly modeled. A 3D representation of uranium with a large grain microstructure is generated using DREAM.3D and a finite element grain model is constructed using a custom tool set. Formation and thickening of a discrete twinned region within the parent grain, which is associated with crystallographic reorientation and characteristic twin shear, is handled with explicit formation and growth of a twin lamella in the finite element framework. To this end, a rigorous procedure is developed for geometry and mesh manipulation associated with twin formation and thickening. Distributions of normalized equivalent and resolved shear stresses are investigated within the parent and twin grain as a function of twin volume in order to elucidate the material response to twin formation and thickening. The calculated mechanical fields are used to determine whether the twin evolution would occur via thickening of the existing twin lamella or formation of a second twin lamella. Furthermore, we analyze the distributions of the most active slip modes. The results suggested that at 5% twin volume fraction, the twin will most likely form a secondary lamella as opposed to continued growth of the first (original) lamella. To our knowledge this is a unique numerical procedure that is able to relate spatially resolved fields of stress, strains with microstructural changes during twin formation and thickening.

Acknowledgements

M.A. wishes to acknowledge support by the G.T. Seaborg Institute for Transactinium Science through the Seaborg Summer Research Fellowship Program. M.K. acknowledges subcontract, NO. 277871, granted by Los Alamos National Laboratory to the University of New Hampshire. I.J.B. and R.J.M gratefully acknowledge support by a Laboratory Directed Research and Development grants 20140348ER and 20140630ER, respectively.
References


Chapter 7

This chapter was published as: Effect of dislocation density-twin interactions on twin growth in AZ31 as revealed by explicit crystal plasticity finite element modeling, Milan Ardeljan, Irene J. Beyerlein, Marko Knezevic, International Journal of Plasticity, 99, 81-101. My role in preparing this chapter was to apply the developed procedure for explicit modeling of discrete twin lamellae within CPFEM to study the effect of dislocation density-twin interactions on twin growth in magnesium alloy AZ31. I performed the modeling work presented in this chapter, post-processed all the necessary data to design and create the figures and graphs that led to important conclusions. Furthermore, I prepared the first draft of the paper and I was actively contributing in producing the final draft along with my co-authors.
Effect of dislocation density-twin interactions on twin growth in AZ31 as revealed by explicit crystal plasticity finite element modeling

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Abstract

In this work, we employ the recently developed framework for the explicit modeling of discrete twin lamellae within a three-dimensional (3D) crystal plasticity finite element (CPFE) model to examine the effects of dislocation densities in the twin domain on twin thickening. Simulations are carried out for \{\overline{1}012\}\{10\overline{1}1\} extension twins in a magnesium AZ31 alloy. The model for the twin lamellae accounts for the crystallographic twin-matrix orientation relationship and characteristic twin shear transformation strain. The calculations for the mechanical fields as a result of twinning consider that one of three types of twin-dislocation density interactions have occurred. One case assumes that the expanding twin retains in its domain the same dislocation density as the parent. The second one considers that twin expansion has lowered the dislocation density as the twin thickens, and the last one, the Basinski effect, assumes that when twin sweeps the region, the dislocation density incorporated in the twin domain is amplified. In the modeling approach, the twin is thickened according to a criterion that maintains the stress state in the vicinity of the grain at a pre-defined characteristic twin resistance. The calculations show that most of the averaged properties, such as the rate of dislocation storage in the entire twin grain, the twin growth rate, the stress field in the twinned grain and neighboring grains, and the slip activity in the parent matrix are not significantly altered by dislocation storage in the twin. The results indicate that, however, the slip activity in the twinned domain is affected. In particular, in
the increased dislocation density case, the rate of dislocation density in the twin domain increases at low strains when the twin is first growing from 2% to 5% volume fraction. This initial boost in the dislocation density storage rate causes the newly expanded dislocation twin to contain more stored dislocations than the other cases for all strain levels. Another interesting difference concerns the preference for one or two twins for the same total twin volume fraction; for the increased dislocation twin or twin that retains the dislocation density as it grows, formation of two twins is favored. For a twin that removes dislocation density, only one twin is preferred. The results imply that in the case with reduced dislocation density leads to lower stored dislocations and dislocation storage rates, and lower pyramidal slip activity.

Keywords: A. Twinning; A. Microstructures; B. Crystal plasticity; C. Finite elements; Dislocation density

1. Introduction

Deformation twinning is an important deformation mechanism, governing both anisotropy and tension-compression asymmetry, as well as texture evolution of many polycrystalline metals, particularly those with low symmetry crystal structures, such as hexagonal (e.g., Mg, Ti, Zr, and its alloys) and orthorhombic (e.g., U). Understanding the effects of deformation twinning on mechanical fields within the grain, its neighbors, and overall material behavior calls for knowledge on how twinning initiates and progresses in time and throughout the grain structure.

Often deformation twinning operates along with dislocation slip as the material is mechanically deformed. How deformation twins propagate is heavily dependent on the interactions between the growing twin lamellae and gliding dislocations. Three main slip-twin interactions, which have been studied via experiment, simulation, and theory, are the volume effect, the barrier effect, and nucleation (Basinski and Basinski, 1989; Beyerlein et al., 2014;
Capolungo et al., 2009; Cheng and Ghosh, 2015; El Kadiri and Oppedal, 2010; Fromm et al., 2009; Jahedi et al., 2017; Kaschner et al., 2006; Knezevic and Landry, 2015; Knezevic et al., 2013b; Knezevic et al., 2013c; Knezevic et al., 2013d; Salem et al., 2003). The first one refers to the lattice reorientation imparted by a twin. The new orientation can alter the preferred slip modes from that of the original parent. The amount of shearing associated with the twin is governed crystallographically by the characteristic twin shear. This value for extension twins in Mg is 0.1289, and thus other deformation mechanisms, such as slip, must be operating in the crystal at the same time. The second one concerns the misorientation imparted at the twin-matrix interface. The alteration in the crystallographic slip planes can pose a barrier to some gliding dislocations. The last one raises the issue of twin nucleation. It has been posed that twins form from slip dislocations (Capolungo and Beyerlein, 2008; Christian and Mahajan, 1995; Mahajan, 2013; Mendelson, 1969, 1970). The latter, in particular, suggests that dislocation glide occurs before as well as during twinning. Taken together, whether twins occur after or during dislocation glide, these issues motivate the questions: what happens to the dislocations stored in the volume of the crystal that later transforms into a twin? How would the fate of these inherited dislocations affect further growth of the twin?

These questions were first addressed by Basinski et al. based on TEM studies of copper (Basinski and Basinski, 1989; Basinski et al., 1997). The Basinski mechanism posits that an increment in strength and/or hardness develops as a result of dislocations changing from glissile parent grain to sessile configurations within twins. It is the geometrical change of dislocation Burgers vector. The mechanism was extended to HCP crystals in (Niewczas, 2010), where the details of vector transformation in those crystals are described. Many works have sought to study this dislocation-twin interaction as twins form and thicken in HCP metals. In studying the
deformation behavior of unalloyed titanium at room temperature, Salem et al. (Salem et al., 2006) revealed two competing effects of deformation twinning on the overall strain-hardening response: strain hardening via the Hall–Petch mechanism (i.e., a reduction in the effective slip length) and the Basinski mechanism. Micro- and nanohardness measurements revealed that deformation twins (immediately after being formed) were harder than the matrix (almost 30%), regardless of the twin thickness and orientation, thus supporting the Basinski mechanism.

El Kadiri and Oppedal (El Kadiri and Oppedal, 2010) proposed the idea of dislocation transmutation. As the parent slips and the twin grows, the twin finds an increasing density of dislocations to incorporate and transmute. The multiplicity of dislocation types in HCP metals, inherited by the twin from the parent, would suggest that the twin stores dislocations more rapidly than the parent. Due to the coherent crystallographic character of the extension twin boundary with parent grain, transmission of dislocations from parent to twin is higher than that to the parent from its neighbors. Additionally, transmutation of dislocations from parent to twin can cause dislocation rearrangements or reconfigurations that leads to dislocation generation. The effect is more pronounced due to the operation of multiple slip modes under deformation of the HCP Mg structure. As such, transmutation results in a higher fraction of dislocation types within the twinned regions than in the parent, forcing them to interact and induce an increasing latent hardening unique for twinning.

Using a 3DXRD experimental technique, capable of tracking the full stress tensor in a grain and an evolving twin, Aydiner et al. (Aydiner et al., 2009) examined the formation of a twin within a parent grain during compression of an AZ31 Mg alloy with the c-axis of the parent grain nearly parallel to the compression axis. The results showed that the stress state in the newly formed twin was lower than that of the parent grain. Using a full-field discrete FFT model,
Kumar et al. (Arul Kumar et al., 2016) were able to explain the reduction in stress by a backstress that develops in the twin via a reaction from the neighboring crystals to the shear of twin. In this work, the effect of dislocation density in the twin or changes in this density before and after twinning was not studied.

Using 3D-XRD, (Bieler et al., 2014) studied strongly textured pure Ti after 1.5 percent tensile strain to nucleate \{10\overline{1}2\} twins. They show that before the twin happens, the stress state in the parent grain is lower prior to twin formation. Apparently, the twin raises the stress in the parent grain after the twin formed. As a further addition to the conclusion made by (Aydıner et al., 2009), they conclude that the deformation history in the neighboring grains also needs to be considered in understanding the stress and strain state of the twin.

Recently, we developed a framework for modeling discrete twin lamellae within a three dimensional (3D) crystal plasticity finite element (CPFE) model (Ardeljan et al., 2015b). The CPFE model accounts for the shear transformation strain and reorientation associated with deformation twinning. These calculations were carried out for twinning in uranium, which has an orthorhombic crystal structure and twins predominantly on the \{130\}\{3\overline{1}0\} systems under ambient conditions. This new technique is a useful tool for studying 3D stress states generated by deformation twin lamellae.

More recently, another approach was developed for modeling discrete twin evolution in polycrystalline microstructures using crystal plasticity finite element framework (Cheng and Ghosh, 2017). The physics of twin nucleation was based on the dissociation of sessile dislocations into stable twin loops, while propagation was assumed to proceed by atoms shearing on twin planes and shuffling to reduce the thermal activation energy barrier. Explicit twinning was accomplished using the evolution of state variables instead of inserting and propagating
twins as separate geometrical objects. The work facilitated modeling of many discrete twins in the microstructure without frequent remeshing. However, the applied plastic strain accommodated by the twin may not have corresponded to the twin volume.

In this work, we apply the technique from (Ardeljan et al., 2015b) to study the generation of 3D stress fields produced by the \{\bar{1}012\}(10\bar{1}1) extension twins in an Mg alloy AZ31. The constitutive law accounts for anisotropic elastic and plastic behavior and uses a hardening law based on thermally activated dislocation density evolution on three modes of slip: basal \langle a \rangle, prismatic \langle a \rangle, and pyramidal \langle c + a \rangle slip. This approach is used to investigate the influence of the twin-dislocation density interactions and the dislocations within the new twin domain that were inherited from the crystalline region before it transformed into a twin after the twin first formed on the driving forces for further growth under mechanical loading.

With the model, we explore the effect of the dislocation density in the twin on the mechanical fields in the crystal as well as the driving forces for further twinning. When the twin is first nucleated and propagated, a twin-dislocation density is assigned point by point within the lamellae. The twin dislocation density is dictated by one of three relationships to the current stored dislocation density at that same point in the volume. The first relation considers one extreme, in which the prior dislocation density is annealed, the second one the other extreme, which is the Basinski effect, wherein the dislocation density is twice as high, and finally the last situation presumes that the dislocation density point for point is unchanged just before and after twinning. With the model, we investigate the three cases of twin thickening on dislocation density storage and their effects on the rate of dislocation storage in the entire twin grain, the twin growth rate, the stress field in the twin and neighboring grains, and the slip activity inside and outside the twin. Interestingly, many of these properties are not significantly altered by how
the twin thickening interacts with stored dislocations. An important effect confirmed here by modeling is that the entire grain with the increased dislocation twin contains more stored dislocations and thus becomes harder as the applied strain is increased. It is also observed that for the same overall twin volume fraction, formation of two twins is more energetically favorable when the density of dislocations within the twin increases or remains constant. On the other hand, formation of a single twin is favored when the overall dislocation density within the twin decreases with applied strain. We examine how the preference for self-thickening of the twin lamella is affected by different dislocation storage rates, stored dislocations, and pyramidal slip activity.

2. Modeling framework

Figure 1 shows a detailed schematic of the multi-level modeling framework utilized in this work. The model evaluates the material response at several length levels going from the right (finer level) to the left side (coarser level). At the coarse length level (frame a) we have the finite element (FE) model where we have introduced the concept of grains. Each grain represents a specific element set that is composed of many finite elements with integration points (frame b). The constitutive response at each integration point is determined by the use of crystal plasticity theory which considers the underlining activity of the crystallographic slip and deformation twinning (frame c) which operate concurrently as the main mechanisms of crystal deformation. As a criterion to initiate twinning, we employ a pseudo-slip model to accumulate the strain to a critical amount (Van Houtte, 1978). Once this criterion is met, we explicitly model the twin lamella(e) by reorienting the lattice and applying the characteristic twin shear. The overall response of the granular microstructural model (polycrystal) is calculated using the finite element homogenization method which satisfies both stress equilibrium and strain compatibility.
conditions (in the weak numerical sense). This model provides a realistic modeling tool for capturing the effects of grain-grain interactions and heterogeneities in the stress-strain fields, all very important aspects when investing the twin-matrix composite.

Other models have been developed for the explicit modeling of a twin lamella in a microstructural framework (Knezevic et al., 2016b; Kumar et al., 2015; Zhang et al., 2008). In these works, the stress fields that develop under relatively small strain levels were studied and hardening was not as critical. In this work, the applied strains will reach moderate levels and the local stresses and strains can grow to be intense. For this reason, the constitutive response employed here includes a hardening law and permits local lattice rotations.

![Figure 1 Schematic of the modeling framework.](image)

The constitutive equations that govern material response are numerically implemented in the User MATerial (UMAT) subroutine and executed in Abaqus Standard. The applied load, prescribed by the appropriate boundary conditions is discretized into increments, where the global stress equilibrium solution is achieved for each and every of the time increments in an
iterative way using the FE method. The finite element governing equation, in its linearized form, that secures stress equilibrium and strain compatibility for each finite element is:

\[(\int_{V} B^T J B \, dV) \Delta U = R - \int_{V} B^T \sigma \, dV.\] (1)

In this relationship, on the left hand side \(B\) stands for FE strain-displacement matrix, \(J\) is material Jacobian matrix, \(\Delta U\) is displacement increment solution, while on the right hand side \(R\) represents the applied force vector and \(\sigma\) is the Cauchy stress tensor (Bathe, 1996).

Below we summarize the constitutive formulation that relates the stress to the strain work conjugate applied at each integration point within each element in the finite mesh (Ardeljan et al., 2014; Kalidindi et al., 1992; Kalidindi et al., 2006; Knezevic et al., 2014d; Savage et al., 2017a; Savage et al., 2017b; Zecevic and Knezevic, 2017; Zecevic et al., 2015b, c). The following notation is used: tensors are denoted using boldface symbols, which are not italic and scalars are denoted using italicized symbols, which are not bold.

2.1. Kinematics of slip and twinning within CPFE

In the description that follows, the main kinematic variables of velocity gradient and deformation gradient are denoted by \(L\) and \(F\), respectively. \(L\) is the sum of the elastic \(L^e\) and plastic \(L^p\) velocity gradients

\[L = L^e + L^p.\] (2)

The \(L^p\) is the sum of the contributions from slip and twinning as follows

\[L^p = L^{sl} + L^{tw}.\] (3)

The velocity gradients for slip and twinning, are given by:

\[L^{sl} = \sum_{\alpha} \gamma^\alpha m^\alpha_0, \quad L^{tw} = \sum_{\beta} \dot{f}^\beta S^\beta m^\beta_0.\] (4)
where \( \dot{\gamma}^\alpha \) is the shear rate on slip system \( \alpha \), \( \mathbf{m}_\alpha^\alpha \) and \( \mathbf{m}_\beta^\beta \) are the Schmid tensors for slip system \( \alpha \) and twin system \( \beta \), respectively, \( S^\beta \) is the characteristic twin shear, and \( N^{sl} \) and \( N^{tw} \) are the total number of available slip and twin systems, respectively. The Schmid tensors are defined as the dyadic product of two orthogonal unit vectors denoting the slip (or twin) shear direction and the slip (or twin) plane normal, respectively. The subscript ‘\( o \)’ denotes that these tensors are known \textit{a priori} and use the initial crystal orientation.

The evolution equation for the twin volume fraction of a given slip system \( \beta \) is given by:

\[
\dot{f}^\beta = \frac{\dot{\gamma}^\beta}{S^\beta},
\]

or in strain increment form,

\[
\Delta f^\beta = \frac{\Delta \gamma^\beta}{S^\beta} \quad \text{(Kalidindi, 1998; Van Houtte, 1978)}.
\]

The complete twin shear strain of 0.1289 is obtained when the volume fraction of a particular extension twin system, \( \beta \), reaches unity, i.e., \( \sum_1^n \Delta f^\beta = 1 \), for a certain number of \( n \) strain increments, and as a result, \( S^\beta = \sum_1^n \Delta \gamma^\beta \).

The total deformation gradient tensor \( \mathbf{F} \) for finite deformations can be decomposed into its elastic and plastic components via:

\[
\mathbf{F} = \mathbf{F}^e \mathbf{F}^p,
\]

where \( \mathbf{F}^e \) contains deformation gradients associated with both elastic stretching and lattice rotation, while \( \mathbf{F}^p \) is the deformation gradient due to plastic deformation alone. The following flow rule relationship is used to define the evolution of \( \mathbf{F}^p \) in a rate form:

\[
\dot{\mathbf{F}}^p = \mathbf{L}^p \mathbf{F}^p, \quad \frac{d\mathbf{F}^p}{dt} = \mathbf{L}^p \mathbf{F}^p.
\]

Integrating Eq. (7) from \( t \) to \( \tau = t + \Delta t \), gives

\[
\mathbf{F}^p(\tau) = \exp(\mathbf{L}^p \Delta t) \mathbf{F}^p(t).
\]

Expressing the exponential as a series and retaining the first order terms yields
\[
F^p(\tau) = \{I + \Delta t L^p\}F^p(t) = \{I + \Delta t(L^{sl} + L^{tw})\}F^p(t),
\]

where \(I\) is the identity matrix. The constitutive equation for the stress in the grain is given by

\[
T^e = CE^e, \quad T^e = F^{-1} \{det F^e\} F^{-T}, \quad E^e = \frac{1}{2}\{F^e T F^e - I\},
\]

where \(C\) is the fourth-order elasticity tensor (Landry and Knezevic, 2015; Wu et al., 2007), \(T^e\) and \(E^e\) are a pair of work conjugate stress and strain measures, and \(\sigma\) is the Cauchy stress for the grain. The elastic deformation gradient \(F^e = FF^{-1}\) is determined by first rewriting Eq. (9) as:

\[
F^{-1}(\tau) = F^{-1}(t)\{I - \Delta t(L^{sl} + L^{tw})\}.
\]

The \(L^{tw}\) is conveniently divided into two parts, \(L^{tw,pts}\) and \(L^{tw,ots}\), i.e.,

\[
L^{tw} = L^{tw,pts} + L^{tw,ots}.
\]

where \(L^{tw,pts}\) is the velocity gradient of the most active variant, or the so-called predominant twin system (pts) and \(L^{tw,ots}\) is the velocity gradient contributed by the other twin systems. Note that every twin system is active in every grain of the polycrystal throughout a plastic deformation process, while continuously accumulating twin volume fraction with plastic strain based on the pseudo-slip model (Van Houtte, 1978). Once the value of accumulated twin volume fraction of a specific twin system (pts) reaches a prescribed threshold value to nucleate or thicken within a given grain, the criterion is met to explicitly propagate or thicken the twin lamella by reorienting the lattice with respect to parent grain and enforcing the characteristic twin transformation shear.

2.2. Kinetics of slip and twinning

To determine the shear strain rate \(\dot{\gamma}^\alpha\), for each slip system \(\alpha\), and \(\dot{\gamma}^\beta\), twinning systems \(\beta\), we use a relationship between the resolved shear stress \((\tau^\alpha = T^e \cdot m_0^\alpha\) for slip and \(\tau^\beta = T^e \cdot m_0^\beta\) for twinning, where ‘\(\cdot\)’ represents the dot product) with their characteristic resistance \((\tau_c^\alpha\) for slip systems and \(\tau_c^\beta\) for twin systems) following a power-law relationship given by (Asaro and Needleman, 1985; Hutchinson, 1976; Kalidindi, 1998):
\[ \dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left( \frac{|\tau^\alpha|}{\tau_c^\alpha} \right)^m \text{sign}(\tau^\alpha), \quad \dot{\gamma}^{\beta} = \begin{cases} \dot{\gamma}_0 \left( \frac{|\tau^\beta|}{\tau_c^\beta} \right)^m \text{sign}(\tau^\beta) & \text{if } \tau^\beta > 0 \\ 0 & \text{if } \tau^\beta < 0 \end{cases} \] (13)

where \( \dot{\gamma}_0 \) is a reference slip rate (arbitrarily set to be 0.001 \( \text{s}^{-1} \)) and \( m \) is a strain rate sensitivity factor (set to be 0.02 for both slip and twinning systems).

For the \( \tau_c^\alpha \) and \( \tau_c^\beta \) evolution, we use the hardening law for AZ31 described in (Ardeljan et al., 2016). The hardening law adopted is a dislocation density based hardening law employing rate equations for dislocation density including thermally activated dynamic recovery. The basic formulation of this particular hardening law dates back to 2008 (Beyerlein and Tomé, 2008) and since then has been adapted for simulation of several low symmetry metal systems including Be (Knezevic et al., 2013a; Zecevic et al., 2015a), Zr (Knezevic et al., 2015b; Zecevic et al., 2016a), Mg (Lentz et al., 2015a; Lentz et al., 2015b; Risse et al., 2017), Ti (Zecevic et al., 2017), and U (Knezevic et al., 2012; Knezevic et al., 2016a; Zecevic et al., 2016b, c) as well as cubic metals (Knezevic et al., 2014a; Knezevic et al., 2014b; Knezevic et al., 2015a; Zecevic and Knezevic, 2015; Zecevic et al., 2016d). The equations are provided in appendix A, while the parameters for AZ31 used in this work are taken from (Ardeljan et al., 2016).

3. Explicit incorporation of twinning in CPFE

3.1. Starting 3D microstructures

We produced a synthetic microstructure using the publicly available software called DREAM.3D, which stands for Digital Representation Environment for the Analysis of Materials in 3D (Groeber et al., 2008; Groeber and Jackson, 2014). Compared to those typically generated via the Voronoi tessellation scheme, DREAM.3D generates grain morphology and grain size distribution that are more realistic. DREAM.3D provides 3D synthetic voxel-based
microstructures and surface meshes for each individual grain based on specified grain size and grain shape distributions. For our interests, we further define voxel density/resolution in the model in order to achieve the desired number of surface finite elements. We use the surface mesh as a bridge between a voxel-based model and a volumetric (in our case tetrahedral) mesh.

The surface mesh is used for 3D mesh generation. Starting from the surface mesh, 3D solid meshing of individual grains is performed to ensure ‘conformal’ grain boundaries in MSC Patran (2013). Conformal boundaries mean mesh conformance between grain boundaries, an aspect that is important when phenomena due to grain-to-grain interactions need to be analyzed, such as stress concentrations at quadruple points. The reader can find a detailed step-by-step explanation of this meshing procedure in (Knezevic et al., 2014c).

3.2. Procedure of incorporating and thickening of twin lamellae in an FE mesh

Explicitly including a twin lamella into the finite element framework required the development of an automated procedure. Hence, scripting capabilities offered in software packages such as Matlab, Patran and Abaqus were successfully employed. This procedure is described in detail in (Ardeljan et al., 2015a; Ardeljan et al.) and consists of several geometric manipulations and mesh generations. For this purpose, we developed a script in Matlab, which writes Patran and Python script files containing specific commands for Patran and Abaqus, respectively. The Patran scripts perform either surface or solid meshing and the Python script files either extract the surface mesh from the solid mesh model or perform the Abaqus mesh cleanup procedure. After this procedure is initially performed in this study, the final result is a twin lamella with a 2% volume fraction inserted with the appropriate crystallographic orientation and shape relative to a selected parent grain that maintains the overall conformity with the parent
and neighboring grains. Further executions of this procedure result in thickening of a priory nucleated and propagated twin lamella according to prescribed twin volume fraction values.

3.3 Procedure for enforcing the characteristic twin shear within reoriented twin lamella volume

So far, we explained all the necessary geometric and FE mesh operations in order to form and thicken the twin lamella. However, to fully model the twin, in addition to the crystal lattice reorientation, intrinsic shearing imposed by creating and thickening twin lamella must be kinematicaly consistent (Ardeljan et al., 2015b). Once the twin lamella is formed, the volume fraction of the predominant twin system ($\beta = tw, pts$) in the corresponding volume reaches unity. To ensure that the strain accommodated by the twin variant $\beta = tw, pts$ corresponds to its volume transferred from the parent either during the twin formation or subsequent thickening, we enforce the twinning shear strain in the twin using

$$
\mathbf{F}^{p^{-1}}(\tau) = \{\mathbf{I} - S^{tw,pts} \mathbf{m}_{0}^{tw,pts}\}.
$$

(14)

Additionally, we ensure that any strain accommodated by the same selected twin variant is removed from the parent grain using

$$
\mathbf{F}^{p^{-1}}(\tau) = \mathbf{F}^{p^{-1}}(t)\{\mathbf{I} + f^{tw,pts} S^{tw,pts} \mathbf{m}_{0}^{tw,pts}\}.
$$

(15)

In the above equations, $f^{tw,pts}$ is the accumulated volume fraction of the selected twin variant in the parent grain. Both Eqs.14 and 15 follow from Eq. 11 and take into account Eq. 5. In summary, Eqs. 14 and 15 enable the required transfer of strain after a twin has formed from the parent to the twin by updating values of $\mathbf{F}^p$ which is simultaneously carried out for all elements belonging to the parent grain and twin.
4. AZ31 twin model

4.1 The model set up

Figure 2 shows the 3D FE microstructural model. This 3D microstructure contains 29 grains and approximately 570,000 finite elements. Each grain consists of roughly 20,000 finite elements. Discretization uses linear tetrahedral elements with one integration point (i.e., type C3D4 in ABAQUS). In order to reveal the interior of the model and to show the grain morphologies, we cut the model in half and expose the two cut planes (see the two right-most images in Fig. 2).

![Figure 2](image)

**Figure 2** A finite element model of explicit grain structure that consists of 29 grains and 570,000 C3D4 elements. The two semi-sections that are perpendicular to each other show the interior of the granular model where the initial crystal orientation of the central grain (colored in green) is set to be favorable for \{\bar{1}012\}〈1\bar{1}01〉 extension twinning for simple compression along the z-direction (ND direction). Note that the models on the left and in the middle are in one, while the model on the right is in a different frame.

We randomly assign crystal orientations to every grain except the green grain in the center of the FE model. The crystal orientation of this grain is selected such that it favors \{\bar{1}012\}〈1\bar{1}01〉 extension twinning under simple compression along the normal direction (ND), i.e. z-direction (Fig. 3). The simple compression is performed by imposing displacement in the z-direction (ND), where the lateral sides are traction-free, and hence free to expand. The compression
consists of several deformation steps, necessary to initially form and then thicken the twin lamella, as will be detailed below. The chosen parent grain orientation is defined by Bunge-Euler angles of \((50°, 95°, 180°)\). The same crystal orientation is assigned to each finite element within each grain, which results in the initial intra-granular misorientations of zero for each grain. Supplementary material of the paper contains the model setup.

![Figure 3](image)

**Figure 3** Distributions of normalized resolved shear stresses \((\bar{R}_{SSTW})\) along the twin plane in the twin direction for all six extension variants after a pre-strain of approximately 0.002 necessary to nucleate initial twin lamella. Normalization was performed with corresponding threshold values for twinning.

For the 3D model grain structure and central grain, once a threshold is reached for twin nucleation, it needs to be inserted, and where it is inserted in the microstructure could have a significant influence on its subsequent growth characteristics. Thus, the key question is where should it form? Twins are a localized phenomenon and not strongly correlated with average properties or average stresses or strains (Christian and Mahajan, 1995). Twins are most likely to
form at points with the highest stress concentration (Bell and Cahn, 1957; Wang et al., 2010a). For the stress concentration component, we elect to use, as a driving force, the resolved shear stress on the twin plane and in the twinning direction (RSSTW) and calculate the stress concentration in RSSTW by considering the value of RSSTW normalized by its critical value, which evolves with deformation and it is governed by dislocation density hardening law. Before moving forward, it is important to keep in mind that the full tensorial fields are calculated at every increment. Should another driving force be deemed more appropriate, it can be easily calculated and used.

Prior to the initial twin lamella formation, a pre-strain of approximately 0.002 in simple compression was applied to a polycrystal along the z-direction. As an implication of a local stress-driven event, it is not necessary that the twin variant with the highest Schmid factor based on the average grain orientation and the applied compression ND load would be the variant that would form. For the purpose of the extension twin variant selection and determining where to insert the twin lamella, we study the RSSTW fields for each of the six extension variants in the grain cluster (Fig. 3). Looking at the central grain alone, we observe that two of the six variants appear to have high RSSTW values with the (011̅2)[0111] variant being the highest and thus we choose to nucleate this variant in the simulations hereinafter. This particular extension twin variant becomes the predominant twin system (fts) as soon as its accumulated twin volume fraction reached a threshold value to form an initial twin lamella. In the present study, the threshold value of 2% is chosen as appropriate. Smaller than 2% is possible to handle by the procedure but is much more challenging to handle as far as geometry and mesh generation due to very small thickness. Due to the specific nature of deformation in AZ31, we see that the neighboring grains could easily deform by twinning as well, but here for simplicity, we carry out
explicit modeling of twin lamella for the central grain only. Note that twinning is allowed in all surrounding grains by employing the pseudo-slip model. Next, the location for the twin lamella of twin variant is determined. As mentioned earlier, it is assumed that favorable twin nucleation sites are found at the grain boundaries at points of highest stress concentration (Bell and Cahn, 1957; Beyerlein et al., 2011; Molnár et al., 2012; Wang et al., 2014; Wang et al., 2010b; Wang et al., 2010c; Zheng et al., 2012). As a measure of determining these stress concentration points we use the von Mises stress values normalized by the applied stress over the entire volume of the grain model (Fig. 4). Figure 4 (a-e) show the contours of normalized von Mises stress values after the pre-strain is applied, while (f-j) show those after the twin propagation. The point of highest stress concentration at the grain boundary of the central grain is indicated by the black arrow. The twin plane location is chosen such that it intersects the volume in the parent grain with the highest twin driving force ($\overline{RSSTW}$) while also connecting the points of the highest stress concentrations found at the parent grain boundaries. Consequently, the exact location will depend not only on the properties of the parent grain, but also on neighborhood orientation and morphology and the applied strain state. Figure 4 also shows contours of normalized von Mises stress values when 2% twin lamella is formed and very small amount of strain is applied (f-j) necessary to establish the stress equilibrium after the twin is inserted. Images show the actual location where the initial twin lamella has been placed. Images (a-c) show different Y-Z sections at constant X of the parent grain before the twin is formed, while (h-j) are the corresponding images after twin lamella is formed. We note that the assumption that twin nucleated at the point of highest stress is not necessarily always the case. The twin partial at the tip near the grain boundary and other slip transfer mechanisms across grain boundaries as well as twin
transmission from grain-to-grain have also been identified as nucleation sites (Wang et al., 2010c).

**Figure 4** Distributions of the von Mises stress normalized by the applied stress over the parent grain without a twin lamella (a-e) and after formation of 2% twin lamella (f-j). Different Y-Z sections of the parent grain at constant X are shown to expose different stress concentration points (without the twin lamella (a-c) and with 2% twin lamella (h-j)). Note that (a) and (h), (b) and (i), and (c) and (j) are the same sections at constant X with each belonging to different strain/time point (i.e. before and after the twin is propagated). Note also that grains shown in (d) and (f) are in a different frame. The black arrow indicates the location of the highest stress concentration.

After forming the twin a choice can be made about the twin dislocation density. Three extreme cases are considered. One involves fully recovering the dislocations within the transforming parent material volume in the twin. Thus the twin-dislocation density is independent of the history of the parent crystal and the strain of twin formation. In the second case, the twin-dislocation density adopts the stored dislocation density at the time of twin formation. In this case, the deformation conditions at the time the twin is first formed affect the
twin-dislocation density. The last case models the Basinski effect, wherein the twin dislocation density is higher than the dislocation density stored in the crystal right before twinning.

To augment the dislocation densities while propagating and thickening the twin, the dislocation densities at the integration points associated with the mesh of the parent are transferred to the integration points corresponding to the mesh of the twin. Only the values in the parent grain located where the new mesh of the twin region exists are altered. In first case, the density in the twin volume increment corresponds to an annealed state \(10^{12} \text{ m}^{-2}\), while the existing twin volume maintains the current heterogeneous dislocation density distribution. The new increment in volume has a homogeneous distribution of dislocation density. In the second and third cases, the dislocation densities can vary from point to point in the increment because the values are based on the current dislocation distribution in the parent transforming to the twin. These assignments to incremental volumes only set the initial dislocation density and with further straining the dislocation density in the twin is allowed to evolve. Appendix B is provided to further clarify the procedure.

4.2 The twinned grain

We first consider effect of a newly formed twin on the stress field of a deformed polycrystal. The new stress field after the twin lamella forms would influence how and where twin growth would initiate. Unless stated otherwise, the instantaneous dislocation density just before twinning is used for the twin-dislocation density. Figure 4 compares the von Mises stress field before and after twinning. We see that the parent stress field in this cross section has not changed substantially and the largest changes occur at the twin tips, where the stress concentrations increase (Fig. 4g). Further, despite the relatively small 2% volume fraction of this newly formed twin, the stress fields in the neighboring grains have been altered. In particular, we see that
relaxation occurs primarily in the neighboring grains that do not intersect the twin. Based on these results, it would seem that the same twin would thicken rather than nucleating a new twin since stress fields along the twin boundary have not dropped or decreased.

To thicken the twin from the initial 2% twin volume fraction, we apply more ND compression to the 3D grain cluster model. The twin is then made to expand in five different deformation steps to volume fractions of 5%, 10%, 20%, 36% and 45%. For the growth step, the FE mesh is altered in a similar manner as twin propagation. Maintaining the same twin normal and location of the initially propagated twin, we cut the surface mesh of the parent grain by two parallel planes with a specified separation in order to expand the twin volume (Fig. 5). In this case, the surface mesh of the parent grain is now reduced for the volume of the previously formed twin lamella. The distance between the cutting planes is changed in order to reflect the twin growth. Appendix B summarizes the procedure. Every time the twin variant propagates, the iterations are performed to ensure that the shear strain accommodated by the twin variant corresponds to its size (Eq. 14) and that the parent grain is free of any strain accommodated by the same twin variant (Eq. 15). In the current modeling approach of explicit twin lamellae, it is not practical to grow its volume every strain increment as the twin accommodates the plastic strain since this would be extremely computationally challenging. We chose the discrete values of twin volume fractions (e.g. 5%, 10%, 20%, 36% and 45%) to facilitate growth of the lamella to a size often observed in AZ31. The sizes of these steps were optimized by considering the distributions of normalized resolved shear stresses (Fig. 9), which is a measure of the driving force to grow a twin. The steps were not made excessively large to influence the parent’s grain propensity to further twin, while they are not too small to unnecessary increase the deformation
steps needed to achieve the target volume fraction (i.e. 45%). We ensured that more frequent increments would not reveal any new phenomena that we did not reveal with the present choices.

Figure 5 Twin propagation and thickening with respect to the surrounding neighboring grains in the 3D model. Grain structure with propagated (a) 2% twin, thickened (b) 5% twin, (c) 10% twin, (d) 20% twin, (e) 36% twin and (f) 45% twin. Different colors are used to highlight the twin thickening increments.

One of the main questions we seek to address concerns the role of the internal twin dislocation density on twin thickening. All calculations below are, therefore, repeated in the case where the dislocation density at integration points associated with the mesh are maintained before twinning (case 1, “the same dislocation twin”), or are reduced to 1 x 10^{12}/m^2 (case 2, “removed dislocation”) or doubled from their current value before twinning (case 3, “the increased dislocation twin”). In prior work (Ardeljan et al., 2015b) the twin-dislocation density was arbitrarily assumed to adopt the current value of the stored dislocation density in the parent at the time of twin propagation and thickening (case 1, same dislocation twin).
Figure 6 compares the von Mises stress fields produced by the twin under load. Since the hardening parameters are adjusted for AZ31, the magnitudes are realistic and thus not normalized. The stresses grow in extent and intensity as the twin grows and the applied strain increases. Many of these details are a consequence of the history of loading, the grain orientations, and the topology of the grain boundary surfaces. With all else being fixed, the comparison shows that the twin volume fraction has the greatest effect on the characteristics of the field, and comparatively, the three twin-dislocation density (DD) situations have relatively small effects. Appendix C shows von Mises contours for the other two cases (i.e. case 2 and case 3). The important point to note is that when the twin dislocation density is removed as it grows, it produces less intense regions of stress. The effect becomes more pronounced as the twin thickens. Thus, whether the twin stores additional dislocations, maintains them, or removes them as it grows, can affect localized stress states not only in the parent grain and the neighboring grain, but the next nearest neighboring grains as well.
Figure 6 Distributions of the von Mises stress (VMises) for different twin volume fractions (same dislocation twin i.e. case 1): (a and a’) 2% twin, (b and b’) 5% twin, (c and c’) 10% twin, (d and d’) 20% twin, (e and e’) 36% twin and (f and f’) 45% twin. In the bottom row (denoted with primed labels) the corresponding parent and twin grains pulled out from the rest of the grains in the cluster are shown.

To thicken the twin, the applied strain is increased, just enough to increase the local stress at the twin/grain boundary junction to rise again. Table 1 presents the twin volume fraction and its corresponding applied strain. As the applied strain increases to 1% and ultimately to 7.5% true strain, the twin in this particular grain thickened from its starting 2% to 45% twin volume fraction.
Table 1 Different aspects of the granular structure relevant to the twin lamella formation and thickening at particular stages of this process.

<table>
<thead>
<tr>
<th></th>
<th>TVF relative to the parent grain x10^-2</th>
<th>TVF relative to the entire FE model x10^-2</th>
<th>Applied effective strain</th>
<th>Effective strain accommodated by the twin</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2.08</td>
<td>0.0969</td>
<td>0.0021</td>
<td>0.0019</td>
</tr>
<tr>
<td></td>
<td>4.91</td>
<td>0.26</td>
<td>0.006</td>
<td>0.0057</td>
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<td></td>
<td>10.07</td>
<td>0.56</td>
<td>0.0127</td>
<td>0.0121</td>
</tr>
<tr>
<td></td>
<td>19.76</td>
<td>1.06</td>
<td>0.0259</td>
<td>0.0241</td>
</tr>
<tr>
<td></td>
<td>35.77</td>
<td>2</td>
<td>0.0489</td>
<td>0.0434</td>
</tr>
<tr>
<td></td>
<td>44.94</td>
<td>2.44</td>
<td>0.0671</td>
<td>0.0558</td>
</tr>
</tbody>
</table>

Figure 7 examines the rate of growth with plastic strain. The case wherein the twin removes dislocation density (DD) grows at a slightly higher rate than the other cases. Once again, the effect of the twin-DD interactions is slight, even when the twin encompasses 45% volume fraction. Figure 8 shows the corresponding total DD (including forest and substructure) development within the twin. When the twin is just 2% volume fraction, the increased dislocation twin increases the rate of dislocation density storage over the other cases. When the twin grows larger than 2%, the effect of twin-DD interactions is negligible. However, as a consequence of the initial boost in storage rate, the accumulated DD in the entire grain is greater in the increased dislocation twin than the “same dislocation twin” or the “removed dislocation twin”.

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Figure 7 Evolution of the twin volume fraction (extension twin) within the central parent grain during simple compression when (a) dislocation densities are transferred from parent to twin region “as is” (same dislocation twin) and (b) the comparison between the three cases with different dislocation density content within the twin region. In the plot 7a different colors are used for different stages (deformation steps) in the process of twin thickening.

Figure 8 Calculated dislocation density in the twin region for three considered dislocation density cases. The results for the total dislocation density in the twinned grain containing two twins are very similar.

The RSSTW stress fields after the twin has thickened at every step are shown in Fig. 9. In every case the RSSTW driving stresses for the same twin system have dropped for regions within the twin lamella, which can be expected since the significant ~86° reorientation has caused other slip systems to be favored.
Figure 9 Distributions of normalized resolved shear stresses along the most dominant twin plane in the twin direction ((01̅2)[0̅111]) for different twin volume fractions before transformation: (a) 2% twin, (b) 5% twin, (c) 10% twin, (d) 20% twin, (e) 36% twin and (f) 45% twin.

Figure 9 can also be used to assess the driving forces for further growth that prevail in the parent grain outside of the lamella. For a more quantitative assessment, we averaged the RSSTW on both twin planes for each twin thickness after transformation. To be more precise, this quantity of averaged RSSTW (normalized twin driving force) was calculated as 

$$\frac{1}{V} \sum_{l=1}^{N_{el}} \frac{\tau_{tw,pts,l}}{\tau_{c,pts,l}} V^l$$

for a prescribed volume of the parent grain, where $tw,pts$ is already defined as the predominant twin system. Figure 10a shows the variation with twin growth in this averaged RSSTW near the twin boundary in the parent. As the twin thickens, the average RSSTW remains close to the CRSS. This serves as validation for the growth criterion and shows that the applied strain was increased just enough to thicken the twin in each case. A similar calculation of the averaged RSSTW is made for the entire matrix volume and the results are shown in Fig. 10b. In this case,
the value begins to decrease as the twin thickens, suggesting that as the twin thickens at the later stages of deformation, more strain would be needed to create a new twin elsewhere and self-thickening becomes increasingly preferred.

**Figure 10** Normalized twin driving force in the central parent grain calculated for different twin volume fractions using two domains: (a) volume close to twin-matrix interface and (b) the entire parent grain. Different colors are used for different stages (deformation steps) in the process of twin thickening.

4.3 **Self-thickening versus two twins**

In the above simulations, the increase in applied work is dissipated by the increase in twin thickness, since the average driving force along the twin plane surfaces is maintained just at the characteristic stress for twinning. We find that the driving force is also maintained in the remainder of the parent grain and only begins to decrease when the twin volume fraction exceeds 35%. Thus, when the twin is still fine (< 35% in volume fraction), the conditions are favorable for forming a second twin in the same grain. Next we apply the model to examine whether twin-DD interactions can affect the preference for achieving the same twin volume fraction by one or two twins.
In the model, as with the first twin, the second twin is formed where the stress concentrations are the highest along the region where the twin boundary intersects the grain boundary. Figure 11 shows the von Mises contour maps for the two twin cases (configurations) for all three types of twin-DD interactions. We find that in this case, the tips of the bottom twin experience a different stress state than the upper twin tips. This can be expected since the two twins have different neighbors and morphologies. Figure 12 shows the slip activity maps. Compared to similar maps for the single twin cases, we observe that having one versus two twins does not substantially affect the slip activity in the matrix (again predominantly basal slip) and in the twin (mixed mode slip of pyramidal, basal and prismatic). Once again, the type of twin-DD interactions has second-order effects on the slip activity in the two-twin cases.

**Figure 11** Two grain structure configurations with parent grain containing (a) one 45% twin lamella and (b) two lamellae, one of 36% and another of 9% volume fraction. Distributions of the von Mises stress contours for all three types of twin-DD interactions are shown.
Figure 12 Distributions of the accumulated shear strains across the whole grain model for basal and prismatic slip systems after equal amount of applied strain of approximately 0.005 with one and two lamellae grain configurations. Accumulated shear strains on basal slip mode in a grain model containing (a) one twin lamella, (b) two twin lamellae and prismatic slip mode with (c) one twin lamella and (d) two twin lamellae. The comparison is also made considering all three types of DD-twin interactions.

The calculation is carried out on both the one twin and the two-twin configurations needed to achieve 45% twin volume fraction. To determine whether one or two twins is more favorable, we incremented the applied plastic strain and calculated the associated increment in strain energy in four volumes: the parent, the twin lamellae, the entire grain (parent + twin), and the entire multi-
grain cluster and considered changes in the plastic work $W_s$, where $s$ represents the number of twin lamellae in the grain model. This change is calculated for the four domains using the relationship $W_s = \frac{1}{V} \sum_1^n \int_V \sigma_{ij} \Delta \epsilon_{ij}^p$, where the increment in plastic strain of 0.005 is applied from the same onset configuration, i.e., the configuration after incrementing either the existing lamella to 45% volume fraction for the one twin case or the configuration after creating the second lamellae without incrementing the existing lamella to 45% volume fraction for the two lamellae case. The results are then compared for each DD-twin interaction case and the difference between the two twin grain configurations is calculated as: $\Delta W = W_1 - W_2$ (Table 2). Table 2 presents calculations of the system energy when the 45% twin volume fraction is embodied in one lamella or two separate lamellae. These results show a remarkable effect of twin-DD interactions. When the stored density is maintained or increased, forming a second twin lamella (with 9% volume fraction) is more energetically favorable than increasing the volume fraction of the original lamella. Although not shown, the twin driving force in the parent grain along the two twin boundaries would lead to the same conclusion. It is just slightly higher in the case of two separate twin lamellae than in the one twin lamella case. However, when the twin removes dislocation density, growth of a single twin is preferred.
Table 2 Comparison of plastic work difference between one lamella and two twin lamellae calculated over the specific volume as indicated in the table.

<table>
<thead>
<tr>
<th></th>
<th>Same dislocation twin $\Delta W \left[ \frac{MJ}{m^3} \right] \times 10^4$</th>
<th>Removed dislocation twin $\Delta W \left[ \frac{MJ}{m^3} \right] \times 10^4$</th>
<th>Increased dislocation twin $\Delta W \left[ \frac{MJ}{m^3} \right] \times 10^4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grain cluster</td>
<td>0.28</td>
<td>-2.06</td>
<td>2.4</td>
</tr>
<tr>
<td>Parent grain + twin</td>
<td>0.29</td>
<td>-0.17</td>
<td>0.4</td>
</tr>
<tr>
<td>Parent grain</td>
<td>0.13</td>
<td>-0.12</td>
<td>0.03</td>
</tr>
<tr>
<td>Twin lamella</td>
<td>0.16</td>
<td>-0.05</td>
<td>0.37</td>
</tr>
</tbody>
</table>

To better understand the preference, we analyzed the dislocation density evolution within the twin lamella and the parent matrix. Figure 13 presents the calculated evolution of the dislocation density on each slip mode (a) within the parent matrix of the twinned grain and (b-d) within the twin lamellae for the three different cases. Despite the preference for basal slip in this alloy, all slip modes are active within the parent matrix and within the twin lamella. For the matrix, basal slip slightly dominates. The selected slip modes in the parent matrix are also not sensitive to how the growing twin affects the stored dislocations and thus it suffices to show the representative calculation in Fig. 13a. We found that the evolution of the dislocation densities in the parent matrix is similar for all three different DD-twin cases that were considered. This suggests that the parent orientation and that of its next nearest neighboring grains largely govern slip activity in the parent. The most interesting difference among the three cases within the twin lamella is that the removed dislocation twin case can be distinguished by a lower dislocation density than the parent and the lowest activity of pyramidal slip among the three cases. We propose that these differences provide an explanation for why self-thickening would be favored over formation of a
new twin for the situation in which twin thickening recovers previously stored dislocations. It has recently been reported that dislocations can readily be transmitted through extension twins in Mg alloys (Molodov et al., 2017). As a result, extension twins in AZ31 could contain a low level of dislocation density. Since extension twins in AZ31 are observed to be thick with majority of grains containing a single or low multiplicity of twin lamellae (Knezevic et al., 2010), our results about the effect of low level of stored dislocations in twin domain on self-thickening is consistent with this new finding about the transmissivity.

Figure 13 Evolution of the dislocation density in (a) the parent matrix and (b-d) the twinned domains for three different dislocation density cases, (b) same dislocation twin, (c) removed dislocation twin, and (d) increased dislocation twin case. There was no significant difference in the dislocation storage rates for the parent matrix in the three cases so (a) is representative of the state of the parent matrix in all three cases. The total DD in (b-d) is the same as in Fig. 8.
5. Conclusions

Using the recently developed framework for explicitly modeling discrete twin lamellae within a 3D crystal plasticity finite element (CPFE) models, we investigated the effects of dislocation density on twin propagation. For a magnesium alloy AZ31 containing \{\overline{1}012\}(10\overline{1}1) extension twins, we calculated the stress fields and analyzed the driving forces for twin growth for three cases of twin dislocation density: full recovery (the twin domain removes the stored dislocation density), maintenance (the twin domain retains it), and the Basinski effect (the twin domain adopts a much larger stored dislocation density, by two times in this case). We show that these cases have little effect on the twin growth rate, the stress field in the twin and neighboring grains, and the slip activity inside and outside the twin. However, we find that the increase in dislocation density content within the twinned region can slow down the twin propagation process and increase the rate of stored dislocations in the entire grain and thus its hardness. The analysis also suggests that when a twin recovers dislocations as it grows self-thickening is preferred over forming a second twin lamella. On the basis of the results here, we propose that this preference occurs when the rate of evolution of dislocation density within the twin is slower than that of the parent.

Acknowledgements

This work is based upon a project supported by the U.S. National Science Foundation (NSF) under grant no. CMMI-1650641. I. J. B. acknowledges financial support from NSF under grant no. CMMI-1728224. Additionally, M.A. wishes to acknowledge the support from the graduate school at the University of New Hampshire through Dissertation Year Fellowship program.
Appendix A

Here, we present for completeness a summary of a dislocation density hardening law formulation used to compute the evolution of slip and twin resistances as a function of strain, temperature and strain rate originally proposed in (Beyerlein and Tomé, 2008).

The resistance for activation of slip considers contributions of several different terms: a friction stress $\tau_{0,f}^\alpha$, a forest dislocation interaction stress $\tau_{for}^\alpha$ and a dislocation substructure interaction stress $\tau_{sub}^\alpha$

$$
\tau_c^\alpha = \tau_{0,f}^\alpha + \tau_{for}^\alpha + \tau_{sub}^\alpha. \quad (A1)
$$

The model for the resistance for twin activation differs from that for slip. It accounts two distinct contributions: a temperature-independent friction term $\tau_0^\beta$ and a latent hardening term coupling the active slip and the twin systems. It is expressed as

$$
\tau_c^\beta = \tau_0^\beta + \mu^\beta \sum_\alpha C^{\alpha\beta} b^\beta b^\alpha \rho_{for}^\alpha. \quad (A2)
$$

Here $\mu^\beta$, $b^\beta$ and $C^{\alpha\beta}$ represent the elastic shear modulus, Burgers vector on the given twin system, and the latent hardening matrix used for coupling, respectively. The behavior of $\tau_{for}^\alpha$ and $\tau_{sub}^\alpha$ is governed by the evolution of the dislocation densities in the form of forest $\rho_{for}^\alpha$ and substructure $\rho_{sub}^\alpha$ dislocations. These relationships, for each dislocation type, can be expressed in the form of a Taylor law

$$
\tau_{for}^\alpha = \chi b^\alpha \mu^\alpha \sqrt{\rho_{for}^\alpha}, \text{ and } \tau_{sub}^\alpha = k_{sub} \mu^\alpha b^\alpha \sqrt{\rho_{sub} \log \left( \frac{1}{b^\alpha \sqrt{\rho_{sub}}} \right)}, \quad (A3)
$$

where $\chi = 0.9$ is a dislocation interaction parameter and $k_{sub} = 0.086$ is a mathematical parameter that insures that Eq. (A3) compensates the Taylor law at low dislocation densities. Since the material is assumed to start in an annealed state, the initial dislocation density in all
simulations was set to $10^{12}$ m$^{-2}$. The stored forest density $\rho_{for}^\alpha$ evolves via a competition between the rate of storage and the rate of dynamic recovery:

$$\frac{\partial \rho_{for}^\alpha}{\partial \gamma^\alpha} = \frac{\partial \rho_{gen,for}^\alpha}{\partial \gamma^\alpha} - \frac{\partial \rho_{rem,for}^\alpha}{\partial \gamma^\alpha} = k_1^\alpha \sqrt{\rho_{for}^\alpha} - k_2^\alpha (\dot{\varepsilon}, T) \rho_{for}^\alpha, \quad \Delta \rho_{for}^\alpha = \frac{\partial \rho_{for}^\alpha}{\partial \gamma^\alpha} |\Delta \gamma^\alpha|, \quad (A4)$$

where $k_1^\alpha$ is a coefficient for the rate of dislocation storage due to statistical trapping of gliding dislocations by the forest obstacles and $k_2^\alpha$ is the coefficient for the rate of dynamic recovery, which is given by the following expression:

$$\frac{k_2^\alpha (\dot{\varepsilon}, T)}{k_1^\alpha} = \frac{x b^\alpha}{g^\alpha} \left( 1 - \frac{kT}{D^\alpha b^2} \ln \left( \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \right) \right). \quad (A5)$$

In Eq. (A5), $k$, $\dot{\varepsilon}_0$, $g^\alpha$, and $D^\alpha$ are respectively Boltzmann’s constant, a reference strain rate, an effective activation enthalpy and a drag stress. Furthermore, the increment in substructure development is proportional to the rate of dynamic recovery of all active dislocations and can be expressed as:

$$\Delta \rho_{sub} = \sum_\alpha q b^\alpha \frac{\partial \rho_{rem,for}^\alpha}{\partial \gamma^\alpha} |\Delta \gamma^\alpha|, \quad (A6)$$

where $q$ is a coefficient defining the fraction of an $\alpha$-type dislocations that do not annihilate but become substructure dislocation. The hardening parameters have been calibrated in the earlier study and used here.

**Appendix B**

This appendix provides a more detailed description of the automated procedure developed for twin lamella incorporation into finite element (FE) mesh. The procedure provides explanation of the necessary steps to initially form a twin lamella in a previously selected parent grain, which can be further thickened with additional straining of the polycrystal (granular microstructure). Additional straining is conducted via a series of consecutive deformation steps resulting in an
incremental increase of the twin’s volume. These deformation steps are necessary, because straining has to be interrupted at specific strain levels to alter the FE mesh and reflect the twin formation and growth. The number of these deformation steps depends primarily on how often polycrystal deformation is interrupted and the amount of twin volume increment used to thicken/grow the twin lamella. In order to better facilitate description of this procedure Figure B1 is shown. Next, the procedure performed between deformation steps to either initially form/propagate or thicken/grow a pre-existing twin lamella in selected parent grain is described.

As previously mentioned, this procedure is made autonomous thanks to scripting capabilities provided in Matlab, Patran and Abaqus software packages. A master script developed in Matlab was used to write appropriate Patran and Python script files with sets of specific commands necessary to be executed in Patran and Abaqus, respectively. Patran was mainly used to perform surface or solid meshing, while Abaqus was used to extract the surface mesh from the solid mesh model or to perform the Abaqus mesh cleanup procedure.

Once the deformation step is accomplished to a certain prescribed strain level (Fig. B1a), procedure starts by obtaining the deformed surface meshes of all individual grains (Fig B1b). This step in the procedure is always performed independently on whether a new twin lamella will be formed first or an existing twin lamella will be thicken for a prescribed volume increment. At this stage, the predominant twin system (pts) and its location have already been determined. Next, either forming (Fig. B1c) or thickening (Fig. B1d) of a twin lamella is performed. Knowing the predominant twin system in the parent grain, the two corresponding twin planes in 3D at specific distance where twin lamella is located in the parent grain can be defined. This distance should reflect the incremental growth of a twin lamella achieved in the previous deformation step. The Matlab script determines the intersection points between these
two twin cutting planes and the 3D surface mesh of the parent grain. The Patran script then uses coordinates of these points to reconstruct the closed loops that define each of the two intersected planes and to mesh them with triangular elements. After the meshing is done, intersection plane surface meshes are exported, which are then used to construct a new parent and twin grain surface meshes. The new twin surface mesh determines the increment in twin’s volume and for each deformation step they are all differently colored, as it is shown in Fig. 5 in the paper. Next, the Matlab script writes a Python script for surface mesh cleanup in Abaqus to collapse any elements with bad aspect ratio. This procedure is performed on a surface mesh of a whole polycrystal. Every triangular element with the edge aspect ratio greater than 4 is been collapsed. Finally, the Matlab script writes an Abaqus input file containing the new mesh, state variables, and boundary conditions for the subsequent deformation step.

**Figure B1** Procedure for explicit incorporation of twinning in CPFE: (a) Deformation step performed in simple compression; (b) Individually deformed surface meshes of all grains. The
intersection between the two twin cutting planes and the 3D surface mesh of the parent grain in the case of (c) twin formation and (d) twin thickening. Differently colored regions (on the right hand side images (c) and (d)) represent the surface mesh of the increment in twin volume.

Appendix C

Figure C1 Distributions of the von Mises stress (VMises) for different twin volume fractions (removed dislocation twin i.e. case 2): (a and a’) 2% twin, (b and b’) 5% twin, (c and c’) 10% twin, (d and d’) 20% twin, (e and e’) 36% twin and (f and f’) 45% twin. In the bottom row (denoted with primed labels) the corresponding parent and twin grains pulled out from the rest of the grains in the cluster are shown.
Figure C2 Distributions of the von Mises stress (VMises) for different twin volume fractions (increased dislocation twin i.e. case 3): (a and a’) 2% twin, (b and b’) 5% twin, (c and c’) 10% twin, (d and d’) 20% twin, (e and e’) 36% twin and (f and f’) 45% twin. In the bottom row (denoted with primed labels) the corresponding parent and twin grains pulled out from the rest of the grains in the cluster are shown.

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Chapter 8

This chapter is currently under review with a title: Explicit modeling of double twinning in AZ31 using crystal plasticity finite elements for predicting the mechanical fields for twin variant selection and fracture analyses, Milan Ardeljan and Marko Knezevic, Journal of the Mechanics and Physics of Solids (submitted). My role in preparing this chapter was to apply and extend the developed procedure for explicit modeling of discrete twin lamellae within CPFEM in order to study the process of formation of a double twin in magnesium alloy AZ31. I performed the modeling work presented in this chapter and I also post-processed all the data to create the necessary figures and graphs that are presented. Furthermore, I prepared the first draft of the paper and I lead in preparing the final draft.
Explicit modeling of double twinning in AZ31 using crystal plasticity finite elements for predicting the mechanical fields for twin variant selection and fracture analyses

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Abstract

A number of studies have found that the formation of double twins in low symmetry metals can lead to the onset of strain localizations, leading further to void nucleation and ultimately fracture. This work extends a recently developed three-dimensional crystal plasticity finite element framework (Ardeljan et al., 2015b) to explicitly model kinematics and kinetics of nucleation/formation, propagation, and thickening/growth of a discrete double twin lamella ($\{10\overline{1}1\} - \{10\overline{1}2\}$) in a magnesium alloy AZ31. With this approach, we model morphological and crystallographic reorientations as well as the shear transformation strains associated with strain accommodation by the double twinning sequence during simple compression and tension. The simulations predict that the distribution of local stress-strain fields during formation and growth of primary contraction twin creates the driving force for the formation of a secondary extension twin variant, which is consistent with experimental observations in both compression and tension. In particular, the contraction twin variant (0111)[0112] is predicted to form an internal extension twin variant (0112)[0111]. Furthermore, the prediction of the underlining crystallographic slip deformation mechanism reveals a substantial activity of basal slip within the contraction portion of the double twin, causing strain localization in its vicinity. Finally, the simulations reveal a gradient in the traction force field across twin-parent interface, suggesting that contraction twin-parent boundaries are weak links in the microstructure where voids can nucleate.
1. Introduction

Magnesium alloys are attractive structural materials for various automotive and aerospace applications due to their light weight and high strength to weight ratio (Cho et al., 2009; Mordike and Ebert, 2001). However, their ductility is limited, which leads to low formability and premature failure at room temperatures (Avedesian and Baker, 1999). Furthermore, magnesium alloys display strong mechanical anisotropy, which is another major hurdle to their widespread use in design and manufacturing (Horst and Mordike, 2006; Hosford and Allen, 1973; Hosford, 2010; Lou et al., 2007). It is thought that the main reason for the lack of ductility of magnesium alloys is the development of $\{10\overline{1}2\} - \{10\overline{1}1\}$ double twins, which promote early shear failure by localized void formation and propagation (Al-Samman and Gottstein, 2008; Barnett, 2007). A significant amount of research has been carried out into reducing and suppressing the development of contraction and double twins in this class of metals by alloying and grain size reduction/refinement (Jahedi et al., 2017; Jain et al., 2008; Lentz et al., 2014; Lentz et al., 2015).

Plastic deformation in polycrystalline metals is most often accommodated by plastic slip, but under certain circumstances it can be carried by both twinning and slip. Magnesium is a hexagonal close packed (HCP) metal which often deforms by twinning in order to accommodate strain along the crystallographic $c$-axis. In Mg alloys, the easiest slip system is basal slip, although prismatic and pyramidal slip systems also operate (Akhtar and Teghtsoonian, 1969; Obara et al., 1973; Roberts, 1960). The most common active twin modes in Mg alloys are extension $\{1\overline{1}2\}\{1\overline{1}1\}$ and contraction $\{1\overline{1}1\}\{1\overline{1}2\}$ modes, where the former facilitates extension and the latter facilitates contraction along the crystallographic $c$-axis (Christian and Mahajan, 1995; Partridge, 1967; Yoo, 1981; Yoshinaga et al., 1973). The $c/a$ ratio for Mg is
1.624 (Barrett, 1952), which is less than the ideal $\sqrt{8/3} \approx 1.633$ for HCP crystal structure. The tension twin mode is easy to activate by applied c-axis tension deformation. Therefore, many experimental reports on various magnesium alloys have shown that extension twins can grow quickly and form thick lamellae, and even encompass the whole grain, and generally reach profuse levels without failing the material (Jiang et al., 2007; Knezevic et al., 2010). In order to accommodate applied strain by activating this type of twinning, crystal structure reorients by $86^\circ$ around $\langle 1\bar{2}10 \rangle$ axis. Overall, these twins can improve ductility, but they lower the strength, due to their relatively low resistance values. On the other hand, contraction twins cause crystal to reorient by $56^\circ$ around $\langle 1\bar{2}10 \rangle$ axis. These twins usually remain very thin and nucleate further a second extension twin inside their domain that often expands very quickly, overtaking most of the contraction twin lamella. As a result, the so-called double twin is formed. It has been experimentally observed that during lateral growth of secondary extension $\{10\bar{1}2\}$ twins, the final $\{10\bar{1}1\} - \{10\bar{1}2\}$ double twin shape is largely enforced by the shape of the primary contraction $\{10\bar{1}1\}$ twin (Barnett et al., 2008b; Cizek and Barnett, 2008).

Experimental characterization of AZ31 samples deformed in tension has been carried out by using transmission electron microscopy. This revealed that c-axis contraction was accommodated predominantly by the formation of $\{10\bar{1}1\} - \{10\bar{1}2\}$ double twins, causing $37.5^\circ \langle 1\bar{2}10 \rangle$ and $30.1^\circ \langle 1\bar{2}10 \rangle$ twin/matrix reorientations (Cizek and Barnett, 2008). The work reported presence of microcracks at the double-twin intersections and locally along the double-twin/matrix interfaces, suggesting that the double-twin formation in polycrystalline Mg alloys promote early shear failure due to localized void formation. In the same work, visco-plastic self-consistent (VPSC) crystal plasticity simulations were employed to aid the interpretation of the obtained results, but the model was unable to fully capture the observed double twinning
sequences. Another study (Beyerlein et al., 2012) sought to explain the nucleation of the secondary twin at the primary twin interface and its early stages of growth in the primary twin domain. The study concluded that the experimentally observed double twinning sequences (Cizek and Barnett, 2008) were more energetically favorable than other sequences.

In many studies (Ando et al., 2014; Barnett, 2007; Cizek and Barnett, 2008; Koike et al., 2010; Reed-Hill and Robertson, 1957; Wonsiewicz and Backofen, 1967; Yoshinaga et al., 1973), the formation of double twins has been correlated to void and crack formation and flow localization in the vicinity of its boundaries. This correlation has been rationalized to arise due to substantial crystal reorientations associated with the double-twinned region and underlining shifts in active crystallographic slip modes. The twin introduces a new crystallographic orientation into the grain and within this domain favorable slip systems may differ from those in the parent. The twinned region of a contraction twin is much more favorably oriented for easy basal slip than the original parent crystal (Beyerlein et al., 2012). The intense basal slip activity that results within the thin lamella region of the double twin produces a localized shear that cannot be accommodated across the primary twin interface and ultimately leads to void formation. Having investigated twinning in a Mg-4wt%Li alloy, (Lentz et al., 2016) recently presented that the lack of plastic relaxation mechanisms causes void formation, especially at the tips of double twin/grain boundary junctions under a complex stress state.

(Niknejad et al., 2016) presented the analysis of transgranular fracture in hot rolled AZ61, which was subjected to triaxial stress state at the vicinity of a notch by combining EBSD and Schmid’s law numerical calculations. Examination of the misorientation boundaries between parent and twin regions discovered a great influence of \{10\overline{1}1\} – \{10\overline{1}2\} double twinning on the formation of transgranular micro-cracks. The study also revealed that this twinning mode
amplifies the shear stresses projected on the basal systems, resulting in early shear localization and transgranular void/crack initiation.

A number of characterization studies showed that the texture changes caused by twinning are the main cause of the observed macroscopic stress–strain anisotropy of HCP metals. In the predominantly slip dominated deformation curves, the hardening rate reduces with applied strain, while in the twinning and slip dominated deformation curves, there are inflection points in the hardening rate, and over some periods the hardening rate increases with applied strain (Knezevic et al., 2013b; Knezevic et al., 2015; Lou et al., 2007). However, the evolution of internal stresses, in a localized stress field in subsets of grains is complex and more challenging to measure. Crystallographic details of a twin can locally affect slip activity and hence influence the macroscopic stress-strain response. Moreover, the directional boundaries introduced by twins can pose obstacles against slip motion and depending on the relative orientation of the slip mode and twin boundary, the barrier effects arise for mobile dislocations. Finally, twin morphology can take affect through the local stress states that are generated within the twin and the surrounding matrix. In addition to creating localized hardening, the localized stress-strain fields produced by twins, also influence the local slip activity within the parent grain and twin itself. They also have an effect on formation of additional twins, and twin expansion rates (Bieler et al., 2014). Knowledge of these local fields can help explain the probability of other twin-governed phenomena, such as secondary twinning and de-twinning (Knezevic et al., 2013a; Morrow et al., 2014; Zecevic et al., 2015a).

The most common crystal plasticity models for metals that deform by a combination of slip and twinning, utilize polycrystal homogenizations, such as Taylor-type (Knezevic et al., 2008; Taylor, 1938) or self-consistent (Lebensohn and Tomé, 1993; Lebensohn et al., 2016). In these
approaches, the grain neighborhood is homogenized and hence the grain boundaries and grain neighbors are not explicitly modeled. Such schemes assume homogeneous stress states in the matrix and twin phases, which can be expected to be very different from the actual highly localized stresses produced by twin domains, as have been reported experimentally using techniques such as far-field 3D-XRD (Abdolvand et al., 2015a; Abdolvand et al., 2015b; Aydiner et al., 2009; Bieler et al., 2014) and differential-aperture X-ray microscopy (DAXM) (Balogh et al., 2013). Localized stresses as a result of twins can be calculated using spatiotemporal models such as phenomenological within FE (Barnett et al., 2013; Zhang et al., 2008), fast Fourier transform crystal plasticity (Kumar et al., 2015), and crystal plasticity finite element (CPFE) (Ardeljan et al., 2014; Ardeljan et al., 2015a; Cheng and Ghosh, 2017). These techniques can calculate the spatially resolved mechanical fields within deformed microstructures, and overcome the limitations of the polycrystal homogenization techniques (Knezevic et al., 2016).

In this work we extend a recently developed crystal plasticity model that explicitly models a twin lamella in 3D in the FE framework (Ardeljan et al., 2015b) to model secondary twin lamellae. The underlining crystal plasticity constitutive model considers both anisotropic elastic and plastic behavior of the material. The implemented hardening law is a function of strain, temperature and strain rate (Beyerlein and Tomé, 2008), and it is governed by the thermally activated dislocation density evolution on three considered slip modes: basal \( \langle a \rangle \), prismatic \( \langle a \rangle \) and pyramidal \( \langle c+a \rangle \). In order to form \{10\(\overline{1}\)1\} − \{10\(\overline{1}\)2\} explicit double twin lamella in the parent grain, we apply plastic deformation such as simple compression or tension to form a primary contraction twin lamella, which after additional straining forms a secondary extension twin lamella within its region. We begin by examining whether the present full-field approach
can predict the most commonly observed double twinning sequence, because such predictions are essential for predicting the local mechanical fields. Unlike in Schmid analysis, the present approach was found successful in predicting the most commonly observed double twinning sequence in both tension and compression. Next, we perform the slip analysis within these regions of interest to determine what slip modes are prevalent. While the formation of an extension twin within an existing twin lamellae is the easiest, basal slip was found to operate more in the remaining portion of the contraction lamellae than within the secondary extension twin. Finally, we investigate the influence of double twinning on the localized stress-strain fields across the granular structure in the vicinity of double twin formation. The simulations reveal a gradient in the field across twin-parent interface suggesting that contraction twin-parent boundaries are locations in the microstructure, where voids can nucleate.

2. Modeling framework

In this section, we present the main relationships and steps in the modeling framework. Figure 1 displays a multi-level modeling framework utilized in this study. Going from left to the right side (frames a-c), the material length magnifies/increases and each frame represents a specific instance at which the material response is being evaluated. At the coarsest level (frame a) we consider the material response of a polycrystal, which is in the form of a granular microstructural model, by the use of finite element (FE) homogenization method. As a full-field model, this method fulfills both stress equilibrium and strain compatibility conditions making it one of the best modeling tools for capturing more realistically the interactions between the constituent grains. Each grain in the polycrystal is represented by an element set, which discretizes a given grain into finite elements (frame b). At this length scale, at each FE integration point, a material constitutive response is being estimated utilizing the crystal
plasticity theory. It assumes that the strain is being accommodated in the material by simultaneous action of crystallographic slip and deformation twinning. The latter is accomplished using the pseudo slip model (Kalidindi, 1998; Van Houtte, 1978). In order to estimate the amount of accommodated shear strain on a particular twin variant plane, a pseudo-slip model is used. Once the prescribed critical twin volume fraction value of a particular twin system is achieved, we explicitly model the twin lamella(e) within the grain, by reorienting the lattice and enforcing the characteristic twin shear. More details about this stage in the modeling procedure are given and discussed in the next section.

![Figure 1](image.png)

**Figure 1** Schematic of the multi-level modeling framework.

In order to determine the single crystal response at each integration point a User MATerial (UMAT) subroutine based on crystal plasticity constitutive formulation was used in Abaqus Standard. The framework facilitates various loading conditions from low to high level of complexity that can be applied in the form of suitable boundary conditions. This applied load is
divided into time/strain increments, where for each and every a global stress equilibrium solution is found using a numerically iterative procedure of the finite element method. This is achieved by solving the Eq. (1), which represents the nonlinear FE governing equation in its linearized form:

\[
\left( \int_{V} B^T J B dV \right) \Delta U = R - \int_{V} B^T \sigma dV.
\]  (1)

In this relation, the listed quantities are respectively \( B \) - finite element strain-displacement matrix, \( J \) - material Jacobian matrix, \( \Delta U \) - displacement increment solution, \( R \) - applied force vector and \( \sigma \) - Cauchy stress tensor (Bathe, 1996; Zecevic et al., 2017; Zecevic et al., 2015b).

Next, we briefly describe the key equations in crystal plasticity constitutive law that we employ in order to relate the material stress to material distortion (stretch plus rotation) at each integration point within each finite element in the model (Kalidindi et al., 1992; Kalidindi et al., 2006). We apply a standard continuum mechanics notation, where tensors are denoted using roman boldface symbols, while scalars are italicized and not boldfaced. To denote a time derivative we place a dot over particular quantity.

2.1 Kinematics of slip and twinning within CPFE

The total velocity gradient tensor, \( L \), can be additively decomposed as following:

\[
L = L^e + L^p,
\]  (2)

where \( L^e \) and \( L^p \) represent elastic and plastic velocity gradients, respectively. The plastic part of the velocity gradient contains the contributions from both slip and twinning via

\[
L^p = L^{sl} + L^{tw}.
\]  (3)

The corresponding contributions to the velocity gradients, due to slip and twinning, are further expressed as:

\[
L^{sl} = \sum_{\alpha}^{N^{sl}} \dot{\gamma}^\alpha m^\alpha_o = \sum_{\alpha}^{N^{sl}} \gamma^\alpha b^\alpha_o \otimes n^\alpha_o, \quad L^{tw} = \sum_{\beta}^{N^{tw}} \dot{f}^\beta S^\beta m^\beta_o = \sum_{\beta}^{N^{tw}} \dot{f}^\beta S^\beta b^\beta_o \otimes n^\beta_o.
\]  (4)
where \( \dot{\gamma}^\alpha \) stands for the shearing rate on the particular slip system \( \alpha \), \( \mathbf{m}_o^\alpha \) and \( \mathbf{m}_o^\beta \) represent Schmid tensors associated with slip system \( \alpha \) and twin system \( \beta \), respectively, \( S^\beta \) denotes the value of characteristic twin shear accompanied to twinning. Finally, \( N^{sl} \) and \( N^{tw} \) represent the total number of available slip and twin systems, respectively. The Schmid tensors represent the unit slip or twin system tensor, defined as the dyadic product \( (\otimes) \) between the unit Burgers direction \( \mathbf{b}_o \) and unit plane normal \( \mathbf{n}_o \) vectors of slip system \( \alpha \) or twin system \( \beta \), respectively, in the undeformed configuration indicated by subscript ‘o’.

In order to determine the rate of change of the twin volume fraction per each particular twin system \( \dot{f}^\beta \), a pseudo-slip model is utilized. This specific model takes under consideration only the shear strain accommodated by twinning and not the morphological and crystallographic reorientation of a twin domain. The latter two are explicitly modeled, as it will be described shortly. The relationship between the \( \dot{f}^\beta \) and the shear rate on the twin system \( \dot{\gamma}^\beta \) is inversely proportional to characteristic shear strain (Kalidindi, 1998; Van Houtte, 1978):

\[
\dot{f}^\beta = \frac{\dot{\gamma}^\beta}{S^\beta}.
\]

Due to integration, in a given strain increment, previous equation becomes:

\[
\Delta f^\beta = \frac{\Delta \dot{\gamma}^\beta}{S^\beta}.
\]

(6)

Integrating over \( n \) strain increments, the accumulated twin volume fraction of a particular twin system, \( \beta \), can reach unity (i.e. \( \Sigma_1^\beta \Delta f^\beta = 1 \)), which means that the particular twin system accommodated the maximum possible amount of shear strain (i.e. \( S^\beta = \Sigma_1^n \Delta \dot{\gamma}^\beta \)).

In our approach, we use a finite deformation formulation, in which an assumption is made that deformation gradient \( \mathbf{F} \) can be multiplicatively decomposed in its elastic \( \mathbf{F}^e \) and plastic \( \mathbf{F}^p \) contributions as:
\[ \mathbf{F} = \mathbf{F}^e \mathbf{F}^p, \]  

where elastic component contains contributions to deformation gradients due to both elastic stretching and lattice rotation, while the plastic component relates contributions to deformation gradients due to plastic deformation. The constitutive relationship between \( \mathbf{F}^e \) and stress in the crystal is made as:

\[ \mathbf{T}^e = \mathbf{C} \mathbf{E}^e, \quad \mathbf{T}^e = \mathbf{F}^{e-1} \{(det \mathbf{F}^e)\mathbf{\sigma}\} \mathbf{F}^{e-T}, \quad \mathbf{E}^e = \frac{1}{2} \{\mathbf{F}^e \mathbf{T} \mathbf{F}^e - \mathbf{I}\}, \]  

(8)

where \( \mathbf{T}^e \) is the second Piola-Kirchhoff stress tensor and \( \mathbf{E}^e \) is the Lagrangian finite strain tensor, both representing a pair of work conjugate stress and strain measures, \( \mathbf{C} \) is the fourth-order elasticity tensor and \( \mathbf{\sigma} \) is the Cauchy stress in the crystal. To compute stress, we need to evaluate the evolution of \( \mathbf{F}^p \) which is ultimately determined by crystallographic slip and twinning (microshear rates) and it can be expressed in a rate form using the following flow rule relationship:

\[ \dot{\mathbf{F}}^p = \mathbf{L}^p \mathbf{F}^p. \]  

(9)

If we integrate Eq. (9) from \( t \) to \( \tau = t + \Delta t \) it becomes:

\[ \mathbf{F}^p(\tau) = \exp(\mathbf{L}^p \Delta t) \mathbf{F}^p(t). \]  

(10)

Furthermore, the exponential can be conveniently approximated and further expanded using Eq. (3) as:

\[ \mathbf{F}^p(\tau) = \{\mathbf{I} + \Delta t \mathbf{L}^p\} \mathbf{F}^p(t) = \{\mathbf{I} + \Delta t(\mathbf{L}^{sl} + \mathbf{L}^{tw})\} \mathbf{F}^p(t), \]  

(11)

where \( \mathbf{I} \) is the identity matrix.

Moreover, we can rewrite previous equation as:

\[ \mathbf{F}^{p-1}(\tau) = \mathbf{F}^{p-1}(t)\{\mathbf{I} - \Delta t(\mathbf{L}^{sl} + \mathbf{L}^{tw})\}. \]  

(12)

Next, we write \( \mathbf{L}^{tw} \) as a summation of two parts:

\[ \mathbf{L}^{tw} = \mathbf{L}^{tw,pts} + \mathbf{L}^{tw,ots}, \]  

(13)
where $L_{tw,pts}$ denotes the velocity gradient of the most active twin variant, which we will be referencing further in the paper as the predominant twin system $(pts)$ and $L_{tw,ots}$ which denotes the velocity gradient from all other twin systems contributing to plasticity.

### 2.2 Kinetics of the slip and twinning mechanism

In order to accurately estimate the amount of shear strain rates, $\dot{\gamma}^\alpha$ and $\dot{\gamma}^\beta$, that can be accommodated at each slip systems $\alpha$ and twinning systems $\beta$, respectively, we use a well establish power-law relationship to compare the resolved shear stress value ($\tau^\alpha = T^e \cdot m^\alpha_0$ for slip and $\tau^\beta = T^e \cdot m^\beta_0$ for twinning) on the system to their corresponding critical resistance value $\tau_c^\alpha$ for slip systems and $\tau_c^\beta$ for twin systems (Asaro and Needleman, 1985; Hutchinson, 1976; Kalidindi, 1998):

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left( \frac{|\tau^\alpha|}{\tau_c^\alpha} \right)^m \text{sign}(\tau^\alpha), \quad \dot{\gamma}^\beta = \begin{cases} \dot{\gamma}_0 \left( \frac{|\tau^\beta|}{\tau_c^\beta} \right)^m \text{sign}(\tau^\beta) & \text{if } \tau^\beta > 0 \\ 0 & \text{if } \tau^\beta < 0 \end{cases} \quad (14)$$

where $\dot{\gamma}_0$ is a reference slip rate (arbitrarily taken here as 0.001 s$^{-1}$) and $m$ denotes the strain rate sensitivity factor (taken here to be 0.02 for both slip and twinning systems).

The hardening law used to govern evolution of $\tau_c^\alpha$ and $\tau_c^\beta$ is presented in (Ardeljan et al., 2016), and it is based on the evolution of dislocation density (DD). In the model, dislocations are stored according to a thermally activated rate law in which the resistances $\tau_c^\alpha$ and $\tau_c^\beta$ are a function of strain, temperature, and strain rate (Beyerlein and Tomé, 2008; Knezevic et al., 2012). These relationships are provided in appendix A for completeness of the present paper. The material parameters for AZ31 utilized in the present model are taken from (Ardeljan et al., 2016).
3. Explicit incorporation of double twin lamella in CPFE

3.1 Finite element model of granular microstructure

In order to create a polycrystal (e.g. Fig. 1a) represented by a cluster of equiaxed grains, a procedure for generation of synthetic granular microstructure is necessary. In this work, the 3D synthetic voxelized microstructure and surface meshes for the grain boundaries were generated in the publicly available software DREAM.3D (Digital Representation Environment for the Analysis of Materials in 3D) (Groeber et al., 2008; Groeber and Jackson, 2014). This software overcomes several limitations of Voronoi tessellation which has been widely used. The generated grains appear more realistic in terms of grain morphology and grain size distribution. Overall, Voronoi tessellation starts with random grain seeds, which create a set of near-equiaxed domains (or grains). It is possible to place these seeds far apart from each other along one dimension in order to get elongated grains, but generally it is difficult to control the grain aspect ratios. Furthermore, since the grain boundary between the two neighboring domains (grains) is always created halfway between the seed points, it proves to be challenging to acquire neighboring grains to be of dissimilar sizes. Finally, one of the main features of Voronoi tessellation is perfectly planar grain boundaries, that might be notably different from real boundaries inferred from microstructure characterization experiments. On the other hand, DREAM.3D can generate 3D voxel-based granular microstructure and surface meshes for each individual grain based on a specified grain size and grain shape distributions. It is also important to mention that DREAM.3D performs a Laplacian based smoothing filter on the voxelized granular microstructure to suppress and remove jagged boundaries between grains which again contributes to better grain representation. A surface mesh consists of triangular elements and represents an important link between a voxel-based model on one side and a volumetric (in our
case tetrahedral) 3D mesh on the other side. Hence, starting from individual grain surface meshes, obtained from DREAM.3D, we developed a meshing procedure to acquire their 3D solid meshes securing mesh conformance between the grain boundaries. This 3D meshing is performed within Patran and the reader can find more elaborate step-by-step description of it in (Knezevic et al., 2014). As a final result of this meshing procedure, we obtain FE model of granular microstructure used in this study. All relevant details concerning the model are provided in the next section (Fig. 3).

3.2 Procedure of discrete double twin lamella modeling

In this section, we summarize steps involved in the procedure for explicit incorporation of twin lamella in FE framework. A reader can find a more in depth explanation of it in (Ardeljan et al., 2015b), where this procedure was developed for the first time. The procedure was later used for explicit formation and thickening of an extension twin lamellae in AZ31 and, in particular, for revealing the effect of dislocation density-twin interactions on twin growth (Ardeljan et al., 2017). The purpose of this study is to explicitly model and investigate a double twin lamella formation in AZ31. The double twin is created within a parent grain by the formation of a primary contraction twin lamella first and then formation of a secondary extension twin lamella within the primary twinned region. This double twin formation is achieved by applying external deformation on the granular microstructure in the form of consecutive deformation steps. The deformation had to be interrupted at specific strain levels in order to alter the FE mesh for the twin formation. Figure 2 is shown to facilitate explanation of the procedure. It shows a brief summary of all intermediate steps necessary to form a twin lamella within the chosen parent grain.
The integrated modeling tool set consists of a master Matlab script that handles post-processing of the deformed granular mesh before and after twin lamella formation and can generate appropriate Patran and Python scripts necessary for performing geometric manipulations and mesh generations. To make this whole procedure as automated as possible, we highly exploited the scripting capabilities of the above mentioned software packages (Matlab, Patran, Python). We execute Patran scripts within Patran, the FE preprocessor from MSC Software, to carry out surface and 3D meshing of individual granular structures once the twin lamella is incepted. On the other hand, Python scripts are used within Abaqus to obtain individual surface grain meshes from the deformed solid granular model (after deformation step is applied) and in the process of mesh cleanup, where bad aspect ratio triangular elements are collapsed before solid meshing of grains in 3D.

After deformation step (e.g. in simple compression) is accomplished to a prescribed strain level (Figure 2a), procedure starts by obtaining the deformed surface meshes of all individual grains (Figure 2b). Next, we want to introduce a twin lamella in the parent grain. At this step, we can assume that predominant twin system (pts) and exact location of the twin lamella in the parent grain are determined. Hence, based on the predominant twin system we can uniquely define in 3D two twin planes on specified mutual distance (Figure 2c). This distance should account for the incremental increase in twin’s volume that accumulated in the previously performed deformation step. The Matlab script identifies all intersection points between these two twin cutting planes and the 3D surface mesh of the parent grain (Figure 2d). Next, the Patran script uses coordinates of these points to reconstruct the closed loops that define each of the two intersected planes and to mesh them with triangular elements of similar size to the ones that build the surface mesh of the intersected (parent) grain. After meshing is done, intersection plane surface meshes are exported, which are then used to construct new parent and twin grain surface meshes (Figure 2e). Finally, Python script performs a mesh cleanup by collapsing any element with aspect ratio greater than 4 in the granular microstructure. This automated procedure is applied after
completion of each deformation step every time when a new twin lamella has to be formed or thickened for a prescribed volume increment. As a final outcome, at the end of this procedure we get a twin lamella of a desired volume incepted into a parent grain with conformal grain boundaries within the granular model.

Figure 2 Procedure for explicit incorporation of twinning in CPFE: (a) An example deformation step of simple compression; (b) Exploded surface meshes of individual grains upon deformation; (c) Intersection between the two twin cutting planes and the 3D surface mesh of the parent grain developing the twin; (d) Two contours composed of intersection points connected by a line used to obtain two meshed twin intersected planes; (e) Resulting twin-parent grain mesh.

While performing the above-mentioned procedure, we tend to reduce as much as possible the changes made to the granular model mesh away from the formed twin lamella region. After meshing the interior of the grains and completing the procedure, in order to transfer the deformation state of all grains in the model from previous step and to use it in the subsequent deformation step, we map the following state variables from the old mesh (before twin lamella inception) to the new mesh (after twin lamella inception): $F^p$ – plastic deformation gradient, dislocation densities and crystal orientations (keeping any developed intra-grain misorientations due to the previous deformation). We map the values of the state variables between the finite
elements in the “old” mesh (before applying any alterations to the mesh) and the “new” mesh (after incepting the twin) based on mutual proximity of their centroids. This element mapping/matching is performed for each grain within the granular model.

From the experimental records it can be inferred that the twin nucleation sites can be usually found at grain boundaries at specific points of highest stress concentration. Hence, the initial location of the primary contraction twin lamella in both cases of simple compression and tension is determined by applying this criterion and examining the von Mises stress contours over the entire volume of the model.

3.3 Accommodation of the characteristic twin shear by twin lamella

Thus far, we described how the morphological and crystallographic reorientation of the twin lamella is handled in our explicit twin modeling approach. Based on a pseudo-slip model and the total accumulated twinning activity a discrete twin lamella of appropriate volume is explicitly formed. However, in order to fully model all aspects of twinning, we also have to account for the accommodation of the characteristic twinning shear within the reoriented twinned volume. Here, we describe the necessary steps that have to be performed in between deformation steps to satisfy the kinematics and kinetics relevant to the twin shear strain, which influences the mechanical behavior of the parent and twin grain before and after the twin lamella is formed.

When the twin lamella is explicitly introduced, regardless of whether it is a primary or secondary lamella, deformation history in both parent and twin grains is updated. This is achieved by modifying plastic deformation gradient ($F^p$) and enforcing the appropriate value at each integration point within each FE belonging to these two regions. In the twinned region, we enforce the values of $F^p$ to be:

$$F^{p^{-1}}(\tau) = \{I - S^{tw,pts} m_0^{tw,pts}\}.$$  \hspace{1cm} (15)
while in the parent grain this value is altered according to:

$$\mathbf{F}_p^{-1}(\tau) = \mathbf{F}_p^{-1}(t)\{1 + f^{tw,pts}S^{tw,pts}m_0^{tw,pts}\}. \quad (16)$$

The accumulated twin volume fraction is denoted with $f^{tw,pts}$, where the superscript denotes the variant $\beta = tw, pts$ that has been selected as previously mentioned predominant twin variant system. These two equations (Eqs. (15) and (16)) ensure the transfer of strain between the parent and twin grain. To be more specific, Eq. (15) assigns the appropriate amount of strain that has been accommodated by the predominant twin variant (pts) to the twin volume, while Eq. (16) ensures that this same amount of strain is deleted from the parent grain. In order to enforce these two equations and retain the numerical stability at the same time, the value of $\mathbf{F}_p$ is multiplicatively decomposed and then updated during much smaller strain (or time) increments at the beginning of each subsequent deformation step. Once the characteristic twin shear transfer is successfully accomplished between the parent and the twin grain, simple compression (or tension) boundary conditions are enforced in order to perform next deformation step to further strain the grain model.

4. Double twinning in AZ31

4.1 Finite element model set up

Figure 3 shows the final FE mesh of the granular microstructure used in this work. We also show the two cut plane views with consistent grain coloring map, where the model is cut in half to expose the interior of the granular microstructure (two right-most images in Fig. 3).
**Figure 3** FE model of explicit grain structure composed of 29 grains and approximately 570,000 C3D4 finite elements. The two semi-sections show the interior of the granular model, where the initial crystal orientation of the central grain (colored in green) is set to be favorable for \(\{10\overline{1}1\}\langle10\overline{1}2\rangle\) contraction twinning.

The created FE model consists of 29 grains in total and approximately 570,000 tetrahedral finite elements (type C3D4 – continuum 3D four nodal). Very fine FE resolution/density is applied, where each grain is discretized with roughly 19,500 finite elements in order to accurately capture inhomogeneity as best as possible in the deformation fields. As mentioned earlier, in the model, twinning is accounted by employing pseudo-slip model. All grains in the polycrystal can deform by twinning, but for the sake of simplicity, we perform explicit modeling of twin lamella for the central grain only. We select the grain positioned in the center of the model which is surrounded by the highest number of grains (colored in green in the two right-most images in Fig. 3) to form a \(\{10\overline{1}1\} – \{10\overline{1}2\}\) double twin. We consider two different deformation modes/scenarios. Therefore, double twin is formed within the central (parent) grain by deforming the granular model, firstly by applying simple compression along the z-axis and secondly by applying simple tension along the y-axis. We arbitrarily allocate crystal orientations in the model for all grains except for the central one, where specific crystal orientation \((0°, 350°, 0°)\), expressed in Bunge-Euler convention, has been assigned for both compression and
tension case. This starting crystal orientation is favorable for \{10\bar{1}1\} contraction twinning for the corresponding deformation cases. Finite elements within any particular grain (element set) share the same crystal orientation. Hence, each grain possesses initial intragranular misorientation of zero degrees. It should be noted that in the tension case, in order to favor contraction twinning over prismatic slip, we lowered the temperature. Hence, deformation in simple tension was simulated at a temperature of 70 K.

The simple compression boundary conditions are prescribed by specifying a displacement of the top surface in the negative z-direction, while enabling the lateral sides to be traction-free and constraining the bottom surface in z-direction. Following the same pattern, simple tension boundary conditions were prescribed by displacing model’s right surface along the positive y-direction. In both deformation cases (compression and tension) double twin was formed in the central grain after applying three consecutive deformation steps. In the first step, the grain model was pre-strained in simple compression to a true strain of 0.073, which was necessary for the parent grain to generate a primary ((0\bar{1}11)[0\bar{1}1\bar{2}]) contraction twin lamella of sufficient volume. This lamella is afterwards explicitly formed. In the subsequent deformation step, the grain model was deformed for additional true strain of 0.056, in order to nucleate a secondary ((01\bar{1}2)[0\bar{1}11]) extension twin within the existing primary twin lamella domain. In the third and final deformation step, the grain model, which now contains the double twin, was deformed for a small additional true strain of 0.015 in order to better reach the equilibrium state after forming the secondary twin and establish stress-strain fields across the volume. These strain increments correspond to the compression case, while the ones for the simple tension case are 0.118, 0.061 and 0.015 respectively. In tension, the same double twin variant sequence (0\bar{1}11)[0\bar{1}1\bar{2}] – (01\bar{1}2)[0\bar{1}11] is predicted as the most favorable. By applying the above mentioned deformation
in the form of three consecutive deformation steps twin lamellae of certain volumes were created. The volume fractions of the primary contraction twin lamellae are 1.5% (compression case) and 1.3% (tension case) of the parent’s grain volume. The percent values represent the volume of the twin lamellae with respect to its corresponding parent grain. In the case of double twin, parent grain of the secondary twin is the primary twinned region/grain. Furthermore, volume fractions of the secondary extension twin lamellae are 49% (compression case) and 50% (tension case) of the primary twin volume. Moreover, the primary twin lamella is formed when the value of accumulated twin volume fraction of the predominant twin system (pts) reaches a threshold value of 1.5% and 1.3% of the central grain’s volume in the case of simple compression and tension, respectively. Likewise, the second deformation step generates the secondary pts of a given volume relative to the volume of the primary twin. After each interruption and each deformation step a transfer of characteristic twin shear between the parent and twin grain is enforced as explained in section 3.3. Next, we explain how these specific primary and secondary twin variants in the central grain were determined along with their corresponding volume fractions.

4.2 Twin variant selection

In order to determine which contraction twin system is the predominant in the parent grain, we look at the distributions of normalized resolved shear stresses $\overline{\text{RSSTW}}$ of all 6 available $\{10\overline{1}1\}{10\overline{1}2}$ contraction twin variants after applying the first deformation step and the pre-strain of 0.073 in simple compression and 0.118 in simple tension. This quantity represents the shear stress resolved on the twin plane and in the twinning direction (RSSTW) that is normalized by its critical value, as entering Eq. (14). Figure 4 displays the interior of the parent grain (y-z cut) and shows these distributions found across it. Furthermore, it represents a driving force for
twin to nucleate, suggesting in which region in the parent grain the twin could initially form. Percent values found below each image show the accumulated twin volume fraction values for the corresponding contraction twin variant. CPFE results show that (0\bar{1}11)[0\bar{1}1\bar{2}] contraction twin is the predominant twin system in the parent grain.

(a)

\begin{align*}
(1\bar{1}01)[1\bar{1}0\bar{2}] & (10\bar{1}1)[10\bar{1}2] & (01\bar{1}1)[01\bar{1}2] & (\bar{1}101)[\bar{1}10\bar{2}] & (\bar{1}011)[\bar{1}01\bar{2}] & (0\bar{1}11)[0\bar{1}1\bar{2}]
\end{align*}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{twin_distributions.pdf}
\caption{Distributions of normalized resolved shear stresses along the twin plane and in the twin direction for all six contraction twin variants after a true pre-strain of: (a) 0.073 in simple compression and (a’) 0.118 in simple tension, which was necessary to nucleate a primary twin lamella. The normalization was performed with the corresponding critical value for onset of twinning. Percentage values indicated at the bottom represent accumulated twin volume fractions per variant at the given strain levels. The sections are made at x=0.5, which cuts the parent grain approximately in half.
}
\end{figure}

When forming primary contraction twin lamella very important question arises; what is the appropriate place where it would form? Twins occur due to highly localized material behavior, not influenced by the average stress or strain properties. Points of the highest stress concentrations in the grain tend to act as favorable twin nucleation sites. These point locations are often, but not necessarily, found at the grain boundaries (Bell and Cahn, 1957; Beyerlein et al., 2011; Molnár et al., 2012; Wang et al., 2010, 2014). In our approach as a measure of
determining stress concentration points in the model we use Von Mises stress values (Figs. 5b, c, b’, and c’). Normalization is performed over the entire volume of the polycrystal with the average value of applied stress. We investigate contours of the normalized RSSTW of (0111)[0112] contraction twin variant, since this variant, as previously defined, is the predominant. Figure 5 contains plots that were used to determine the exact location where the primary contraction twin lamella (1.5% and 1.3% of the parent volume fraction in compression and tension respectively) was formed. The lower right part of the parent grain was selected as the most favorable location for twin to nucleate, since it is the region of the highest stress concentration and also has a large driving force to from the twin (Figs. 5a, b, a’, and b’).

![Figure 5](image_url) Distribution of normalized resolved shear stresses (RSSTW) for (0111)[0112] predominant contraction twin variant after a pre-strain of (a) 0.073 in simple compression and (a’) 0.118 in simple tension. Distributions of von Mises stress normalized by its average value over the granular microstructure: (b) right before and (c) after the formation of 1.5% primary
contraction twin lamella in simple compression and (b’) right before and (c’) after the formation of 1.3% primary contraction twin lamella in simple tension.

Furthermore, after performing the second deformation step, we found that roughly 50% of the twin volume fraction was accumulated (according to the pseudo-slip model for twinning) on predominant (01\overline{1}2)[0\overline{1}11] extension twin variant plane within the previously incepted primary twin volume. Figure 6 displays contours of RSSTW across the primary twin lamella for all 6 available \{10\overline{1}2\}{10\overline{1}1} extension twin systems. The contours are shown on both sides of the primary contraction twin volume. It shows a tendency of forming (01\overline{1}2)[0\overline{1}11] extension twin lamella inside the primary twin region. Furthermore, explanation of the double twin classification into different types is provided in the following section.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6.png}
\caption{Distributions of normalized resolved shear stresses along the twin plane and in the twin direction for all six extension variants after the second deformation step to an additional true strain of: (a) 0.056 in simple compression and (a’) 0.061 in simple tension, which was required to nucleate a secondary twin lamella. The normalization was done with a corresponding critical value of twin resistance values for onset of twinning. For each twin variant both sides of the primary twin lamella are shown. Percentage values indicated at the bottom represent accumulated twin volume fractions for each extension twin system at the given strain level.}
\end{figure}
Finally, Fig. 7 shows views of the granular microstructure and the central grain after each deformation step necessary to form a double twin in simple compression and tension. Once the 50% secondary extension twin lamella was incepted, the volume of the initial primary contraction twin lamella was not changed. This is justified, because in the lateral growth of secondary \( \{10\bar{1}2\} \) twins, the final shape of a double twin is mainly enforced by the shape of primary \( \{10\bar{1}1\} \) twin (Barnett et al., 2008b; Cizek and Barnett, 2008).

Figure 7 Double twin formation during simple compression (top row) and simple tension (bottom row) with respect to the surrounding neighboring grains in the 3D granular microstructure. (a and a’) Initial microstructure, where the central grain colored in green, is favorably oriented for \( \{10\bar{1}1\}\{10\bar{1}2\} \) contraction twinning. (b and b’) Granular microstructure after the formation of the \( (0\bar{1}1\bar{1})[0\bar{1}1\bar{2}] \) primary contraction twin in the parent grain. (c and c’) Granular microstructure upon double twin formation, where the secondary extension twin lamella \( (01\bar{1}2)[0\bar{1}1\bar{1}] \) is colored in light blue. The unprimed and primed labels are for simple compression and simple tension, respectively.
4.3 CPFE vs. Schmid analysis of primary and secondary twin variants

In general, the material response is highly affected by the rapid reorientation of crystallographic texture due to primary and secondary twinning (Ando et al., 2010; Barnett et al., 2008a; Niknejad et al., 2016). Therefore, an accurate prediction of the most dominant twin variants that occur in the microstructure is of high importance. The most commonly adopted method that has been used to investigate the mechanism of primary and secondary twin variant selection under different loading conditions is Schmid factor analysis (Godet et al., 2006; Xin et al., 2014). Recent statistically significant experimental findings suggest that behavior of AZ31 Mg alloy deviates from Schmid-like behavior for both primary and secondary twinning (Abdolvand et al., 2015a; Barnett et al., 2008b). This type of behavior usually represents an implication of a locally stress-driven event, when the local stress state in the grain is significantly different from the macroscopically imposed stress state.

We provide a brief background about the two step twin variant sequence that occurs during the process of double twinning. We focus on the particular double twin variant sequence observed in AZ31 during both simple compression and tension using our 3D CPFE modeling approach which explicitly models double twin lamella. We also provide misorientation relations between the original parent (matrix) and doubly twinned volumes.

In terms of twinning in AZ31, we have six contraction and six extension twin variants. In order to form a double twin, each of the six contraction twin variants (cause primary twin reorientation of ~56° around a \(\langle 1\bar{2}10 \rangle\) axis) can form/nucleate one of the six available extension twin variants (secondary twin reorientation of ~86° around a \(\langle 1\bar{2}10 \rangle\) axis). Hence, in the most general case double twin formation covers 36 different primary-secondary pairs of twin variants (Martin et al., 2010). However, all of them can be classified into only four groups (types)
depending on the overall reorientation that they cause with respect to the parent/matrix crystal orientation. Based on our CPFE predictions in both simple compression and tension cases same double twin variant sequence is predicted. As already stated, the primary predominant contraction twin variant is \((0\bar{1}11)[0\bar{1}1\bar{2}]\), while the secondary predominant extension twin variant is \((01\bar{1}2)[0\bar{1}11]\). More detailed visual representation of the above mentioned twin variants is shown in Figure 8 where red color markers were used to tag these twin variants. Furthermore, Table 1 classifies twin variants into 4 different types, also containing the corresponding misorientation relationships. According to this table the developed double twin can be classified as type 2, which is along type 1 usually expected to form in compression along an axis close to the c-axis (Barnett et al., 2008b).

**Figure 8** Stereographic projection of the basal \{0001\} pole of the initial parent orientation, 6 contraction (primary) and 6 extension (secondary) twin variants. Red colored markers are used to denote the specific twin variants (the predominant twin systems), which are modeled using CPFE as a primary and a secondary twin variant. Secondary extension twin variants \((f1-f6)\) reorient from the primary contraction twin variant denoted with red star, F.
Double twin variants | $f_1$ (type 1) | $f_4$ (type 2) | $f_2$ and $f_3$ (type 3) | $f_5$ and $f_6$ (type 4)  
--- | --- | --- | --- | ---  
Misorientation | 37.5° | 30.1° | 66.5° | 69.9°  

**Table 1** Six $\{10\overline{1}1\} - \{10\overline{1}2\}$ double twin variant pairs classified into 4 types. Misorientation angles about the common zone axis between the basal planes of the matrix/parent define the 4 different double twin types.

Furthermore, we provide Schmid factor analysis for basal slip systems, contraction and extension twin variant systems under simple compression and tension. We consider crystal orientations in the parent region, as well as in the double twin region. The results of the analysis are presented in Table 2. Schmid factor of a specific crystallographic system (slip or twin) can be computed as the ratio between the shear stress that can be resolved on the particular slip or twin plane and the macroscopic stress state that is imposed to evaluate the $(\tau)$ in the crystal or more conveniently expressed using the angles:

$$M = \frac{\tau}{\sigma} = \cos \lambda \cdot \cos \phi.$$  

(17)

The angles $\lambda$ and $\phi$ represent angles between the loading axis and the crystallographic plane normal and direction vectors, respectively, for each specific crystallographic system. Red stars are put in the table next to the most stressed twin variant systems determined by the analysis. Also, we assume that the macroscopic stress ($\sigma$) of unity (1 MPa) was applied for both simple compression and tension cases, to estimate resolved shear stress for each crystal orientation. Due to the directionality of the twinning, twin variants can be activated only if the resolved shear stress (or Schmid factor) is positive.

In compression, results of the Schmid analysis match well the results obtained from our 3D CPFE modeling approach. In fact, the most heavily stressed twin systems (highest Schmid factor-marked with a red star in Table 2) are found to be the most dominant ones in the CPFE simulations (marked with a blue star in Table 2). However, in the tension case, twin variant
selection slightly deviates from the Schmid-like behavior, because the secondary predominant extension twin variant system does not have the highest Schmid factor value. The Schmid analysis predicts the rarely observed type 3 sequence. Interesting observation which we find important to note here is that in simple tension all 6 available extension twin variants possess relatively high and similar Schmid factor values.

<table>
<thead>
<tr>
<th>Schmid factor values</th>
<th>Compression</th>
<th>Tension</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>parent twin</td>
<td>secondary twin</td>
</tr>
<tr>
<td>3 basal systems</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(0001)[21\bar{1}0]</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(0001)[\bar{1}2\bar{1}0]</td>
<td>-0.148</td>
<td>0.32</td>
</tr>
<tr>
<td>(0001)[\bar{1}120]</td>
<td>0.148</td>
<td>-0.32</td>
</tr>
<tr>
<td>6 contraction twin variants</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\bar{1}101)[\bar{1}102]</td>
<td>0.447</td>
<td>-0.122</td>
</tr>
<tr>
<td>(10\bar{1}1)[10\bar{1}2]</td>
<td>0.352</td>
<td>0.083</td>
</tr>
<tr>
<td>(01\bar{1}1)[01\bar{1}2]</td>
<td>0.295</td>
<td>-0.075</td>
</tr>
<tr>
<td>(\bar{1}101)[\bar{1}102]</td>
<td>0.352</td>
<td>0.083</td>
</tr>
<tr>
<td>(\bar{1}011)[\bar{1}012]</td>
<td>0.447</td>
<td>-0.122</td>
</tr>
<tr>
<td>6 extension twin variants</td>
<td></td>
<td></td>
</tr>
<tr>
<td>f1 (0\bar{1}12)[01\bar{1}1]</td>
<td>-0.458</td>
<td>0.312</td>
</tr>
<tr>
<td>f2 (1\bar{1}02)[\bar{1}011]</td>
<td>-0.486</td>
<td>0.035</td>
</tr>
<tr>
<td>f3 (\bar{1}02)[1\bar{1}01]</td>
<td>-0.486</td>
<td>0.035</td>
</tr>
<tr>
<td>f4 (01\bar{1}2)[0\bar{1}11]</td>
<td>-0.480</td>
<td>0.361**</td>
</tr>
<tr>
<td>f5 (\bar{1}012)[1\bar{1}01]</td>
<td>-0.475</td>
<td>0.011</td>
</tr>
<tr>
<td>f5 (\bar{1}\bar{1}02)[\bar{1}\bar{1}01]</td>
<td>-0.475</td>
<td>0.011</td>
</tr>
</tbody>
</table>

Table 2 Calculated Schmid factor values for basal slip, contraction, and extension twin variants within parent, primary, and secondary twinned regions under simple compression and simple
tension. The most heavily stressed twin systems based on the Schmid analysis are tagged with red stars, while those based on the CPFE simulations are tagged with blue stars. The relevant labels of twin variants in the most left column are consistent with those in table 1 and Fig. 8.

5. Stress fields as predicted by CPFE

Figure 9 shows the evolution of von Mises stress fields across the granular microstructure as double twin forms during simple compression and tension deformation steps. Material parameters used in the dislocation density hardening law were calibrated for AZ31 to capture its material response across large range of different strain rates and temperatures (Ardeljan et al., 2016). Hence, the showed stress magnitudes are realistic and are not normalized. As more strain is applied, double twin forms in the parent grain interior, which is followed by the increase in stress magnitude in the vicinity of the formed double twin. It is noticeable that this event governs stress distribution in some of the neighboring grains as well. These specific details are governed by the particular grain orientations, morphology of the grain boundary surfaces, and history of loading.
Figure 9 Distributions of von Mises stress at different stages of double twinning: (a and a’) right before (\(0\overline{1}11\))[\(\overline{0}\overline{1}1\overline{2}\)] primary contraction twin formation (end of the first deformation step), (b and b’) right before (\(01\overline{1}2\))[\(\overline{0}\overline{1}11\)] secondary extension twin formation (end of the second deformation step), and (c and c’) upon double twinning and a small amount of additional deformation of 0.015 true strain (end of the third deformation step). The unprimed and primed labels are for simple compression and simple tension cases, respectively.

Furthermore, we investigate how plastic strain is accommodated across the granular microstructure as external deformation is applied. Figure 10 shows strain concentration distributions (\(\text{PEEQ}\) - equivalent plastic strain is normalized with the applied strain) after primary and secondary twin lamellae have been introduced. The shown plots correspond to the deformation states after the second and third deformation steps in simple compression and tension. An interesting conclusion can be drawn that most of the strain is contained in the primary contraction twin lamella region. This state remains even after secondary twin lamella is formed. Figure 11 can explain this kind of behavior by providing the distributions of the
accumulated shear strains for basal and prismatic slip modes for the corresponding deformation steps. These values are plotted at the end of each performed deformation step ensuring the same strain levels. These slip activity maps show the amount of basal and prismatic shear strains accumulated in each of the three deformation steps that were carried out for the corresponding externally applied strain increments. Hence, for each deformation step these values start from zero and accumulate as the external deformation is applied. The double twin region is favorable for basal slip due to the twin induces crystal reorientation. Moreover, the highest activity of the basal slip mode is observed within the primary contraction twin lamella.
Figure 10 Distributions of normalized value of equivalent plastic strain (PEEQ) (a) right before and (b) after secondary twin formation in simple compression and (a’) right before and (b’) after secondary twin formation in simple tension. Note that in (b) and (b’) a small amount of additional deformation of 0.015 true strain was applied upon double twinning. The inserts show the contours across primary contraction and secondary extension portions of the double twin. The normalization is performed by the applied equivalent plastic strain value.
Figure 11 Distributions of the accumulated shear strains across the whole grain model for basal and prismatic slip modes: (a and a’) right before primary contraction twin formation (end of the first deformation step), (b and b’) right before secondary extension twin formation (end of the second deformation step), and (c and c’) upon double twinning and a small amount of additional deformation of 0.015 true strain (end of the third deformation step). The unprimed and primed labels correspond to simple compression and simple tension cases, respectively. Note that the
values are initialized before a given deformation step and reflect those accumulated during the given deformation step.

In order to better understand the inhomogeneity introduced by formation of double twin, we examine distributions of traction forces at the double twin-parent boundary. This boundary is initially introduced by the formation of the primary contraction twin lamella and, subsequently modified by secondary twinning to consists of two crystallographically different parts, where parent and either contraction or extension twin meet. Figure 12 shows the distributions of traction force magnitude that are spatially resolved across twin-matrix boundaries at the end of the second and the third deformation steps in simple compression and tension. Both sides of the double twin-parent boundary are shown (i.e. from twin’s and parent’s side). The field on the parent side is calculated from stress in the finite element layer of the parent adjacent to the interface ($\sigma^{\text{parent}}$), while the field on the twin size is calculated from stress in the element layer in the twin adjacent to the interface ($\sigma^{\text{tw}}$). Traction force vector is obtained as a projection of the Cauchy stress tensor in each finite element on the twin lamella normal and its magnitude is calculated using: $|\mathbf{f}| = |\sigma \cdot \mathbf{v}^{\text{tw,pts}}|$, as schematically shown in Fig. 13. Note that the vector $\mathbf{v}^{\text{tw,pts}}$ is conveniently defined to locally change its direction over the interface as it always points from the twin to the parent, unlike the crystallographic plane normal $\mathbf{n}^{\text{tw,pts}}$. Existence of the spatial gradient in the magnitude of the traction force across and over the interface indicates that fracture could initiate from the twin-matrix interface.
Figure 12 Distributions of magnitude of traction force across the twin-parent boundary: (a and a’) right before secondary extension twin formation (end of the second deformation step) and (b and b’) upon double twinning and a small amount of additional deformation of 0.015 true strain (end of the third deformation step). Both sides of the twin-parent boundaries are shown. The unprimed and primed labels are for simple compression and simple tension, respectively.

Figure 13 Schematic of the twin-matrix boundaries showing the vector $v^{tw,pts}$ pointing from twinned region to its surrounding.
The magnitude of the traction force shown in Fig. 12 lacks the information of acting direction. Figure 14 shows the difference in traction force at the twin-parent interface (i.e. between the parent and the twin side of the interface) in the direction pointing from the twinned region towards the parent surrounding (Fig. 13). It is computed using the relationship:

$$\Delta f = f_{\text{parent}} \cdot \mathbf{v}_{\text{tw} \cdot \text{pts}} - f_{\text{twin}} \cdot \mathbf{v}_{\text{tw} \cdot \text{pts}}.$$  

The difference between traction forces in this particular direction, $\mathbf{v}_{\text{tw} \cdot \text{pts}}$, further confirms the heterogeneity in the field created by double twinning that can lead to void initiation and propagation to failure. Variation in the tensile and compressive sense of the traction forces along the $\mathbf{v}_{\text{tw} \cdot \text{pts}}$ direction is the highest along the primary contraction twin-parent boundary for both simple compression and tension cases. In particular, the predicted tensile traction region points to void formation from the twinned region, as experimentally observed in (Barnett, 2007). The voids were observed to either consume a significant portion of the twinned region or sometime even to form in the twin interior. In summary, the presence of strong traction force gradient of even variable sign suggests that twin-parent interface is a favorable void nucleation site in the microstructure. Future work will consider the implementation of cohesive zone elements at the twin-parent interface to facilitate modeling of interface decohesion.
6. Summary and conclusions

We have extended a recently developed CPFE framework for explicit modeling of microstructure to model a discrete double twin lamella. The present study is applied to a magnesium alloy AZ31, an HCP material that deforms by a combination of crystallographic slip and deformation twinning, and has a tendency of forming double twins. These twins are experimentally found to lead to a void formation and failure of AZ31. A polycrystal in the form of synthetically generated granular microstructure was studied in simple compression and tension. Centrally located grain in the microstructure surrounded by the largest number of

![Figure 14](image_url)
neighboring grains was chosen to form a double twin lamella. The lamella was developed by executing three consecutive deformation steps consisted of pre-straining (to form a primary contraction twin), followed by straining (to form a secondary extension twin), and finally a small amount of additional deformation upon double twinning. While all constituent grains in the microstructure were allowed to deform by slip and twinning, the explicit modeling of a twin lamella was performed only for a suitably oriented central grain. The model successfully predicts the most commonly observed “double twin” sequence, \((0\bar{1}11)[0\bar{1}1\bar{2}] - (0\bar{1}1\bar{2})[0\bar{1}11]\), as the most likely to occur in both simple compression and simple tension. The predicted sequence in the parent grain obtained using the CPFE simulations in simple compression match well the corresponding results of the Schmid analysis. In contrast, in the tension case, the twin variant selection based on CPFE deviated from the one based on the Schmid analysis. The stress fields predicted by CPFE govern the correct sequence. Furthermore, the predicted stress fields in the microstructure with the double twin reveal concentrations more in the close vicinity of the initially formed primary contraction twin than in the secondary twin. The primary contraction twin region was predicted to deform by a large amount of basal slip. Finally, the investigation of the traction forces acting on a double twin-parent interface reveals that the contraction twin-parent interface is a weak link in the microstructural grain boundary network, which is susceptible to void nucleation.

**Acknowledgements**

This work is based upon a project supported by the U.S. National Science Foundation (NSF) under grant no. CMMI-1650641. M. A. also wishes to acknowledge the support from the graduate school at the University of New Hampshire through Dissertation Year Fellowship program.
Appendix A

For completeness of the presented constitutive model, we provide a summary of the utilized dislocation density hardening law. This formulation of the hardening law was used to compute the evolution of slip and twin resistances as a function of strain, temperature, and strain rate (Ardeljan et al., 2017; Beyerlein and Tomé, 2008).

In order to estimate the resistance required to trigger slip, we take into account the contributions of the following terms: a friction stress $\tau_{0,f}^\alpha$, a forest dislocation interaction stress $\tau_{for}^\alpha$ and a dislocation substructure interaction stress $\tau_{sub}^\alpha$:

$$\tau_c^\alpha = \tau_{0,f}^\alpha + \tau_{for}^\alpha + \tau_{sub}^\alpha.$$  \hspace{1cm} (A1)

The resistance for twin activation evolves considering a temperature-independent friction term $\tau_0^\beta$ and a latent hardening term which performs coupling between the active slip and twin systems. Accounting for both effects, the resistance for twinning is expressed as:

$$\tau_c^\beta = \tau_0^\beta + \mu^\beta \sum\alpha C^{\alpha\beta} b^\beta b^\alpha \rho_{for}^\alpha.$$ \hspace{1cm} (A2)

In this relationship $\mu^\beta, b^\beta$ and $C^{\alpha\beta}$ represent respectively the elastic shear modulus, Burgers vector on the given twin system, and the latent hardening matrix used for coupling. Furthermore, the individual behavior of $\tau_{for}^\alpha$ and $\tau_{sub}^\alpha$ is determined by the evolution of the dislocation densities that consist of forest $\rho_{for}^\alpha$ and substructure $\rho_{sub}^\alpha$ dislocations. For this purpose a Taylor-like law is used to represent these relationships for each dislocation type. These are expressed as:

$$\tau_{for}^\alpha = \chi b^\alpha \mu^\alpha \sqrt{\rho_{for}^\alpha},$$ \hspace{1cm} (A3)

$$\tau_{sub}^\alpha = k_{sub} \mu^\alpha b^\alpha \sqrt{\rho_{sub}} \log \left( \frac{1}{b^\alpha \sqrt{\rho_{sub}}} \right).$$ \hspace{1cm} (A4)

Here $\chi$ is a dislocation interaction parameter set to 0.9 and $k_{sub} = 0.086$ is a mathematical parameter that insures that Eq. (A3) compensates the Taylor law at low dislocation densities.
(Capolungo et al., 2009). The initial material state corresponds to an annealed state, hence the initial dislocation density was set to $10^{12}$ m$^{-2}$. The value of stored forest density $\rho_{for}^\alpha$ changes according to competition between the rate of storage/generation and the rate of dynamic recovery/removal:

$$\frac{\partial \rho_{for}^\alpha}{\partial \gamma^\alpha} = \frac{\partial \rho_{gen,for}^\alpha}{\partial \gamma^\alpha} - \frac{\partial \rho_{rem,for}^\alpha}{\partial \gamma^\alpha} = k_1^\alpha \sqrt{\rho_{for}^\alpha} - k_2^\alpha (\dot{\varepsilon}, T) \rho_{for}^\alpha, \quad \Delta \rho_{for}^\alpha = \frac{\partial \rho_{for}^\alpha}{\partial \gamma^\alpha} |\Delta \gamma^\alpha|. \quad (A5)$$

In Eq. (A5) $k_1^\alpha$ is a coefficient for the rate of dislocation storage because of statistical trapping of gliding dislocations and $k_2^\alpha$ is the coefficient for the rate of dynamic recovery by thermally activated mechanisms. The second coefficient can be determined by this relationship:

$$\frac{k_2^\alpha (\dot{\varepsilon}, T)}{k_1^\alpha} = \frac{\chi b^\alpha g^\alpha}{\gamma^\alpha} \left( 1 - \frac{kT}{D^\alpha b^\alpha} \ln \left( \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \right) \right), \quad (A6)$$

where $k$, $\dot{\varepsilon}_0$, $g^\alpha$ and $D^\alpha$ are respectively Boltzmann’s constant, a reference strain rate (taken here to be $10^7$ s$^{-1}$), an effective activation enthalpy and a drag stress. Lastly, the increment in substructure development can be related to the rate of dynamic recovery of all active dislocations as:

$$\Delta \rho_{sub} = \sum_\alpha q b^\alpha \frac{\partial \rho_{rem,for}^\alpha}{\partial \gamma^\alpha} |\Delta \gamma^\alpha|, \quad (A7)$$

where $q$ is a rate parameter that determines the fraction of an $\alpha$-type dislocations that do not annihilate, but become substructure dislocation. As previously mentioned in the text, the material parameters used in this hardening law have been calibrated in a prior study.
References


Zecevic, M., Beyerlein, I.J., Knezevic, M., 2017. Coupling elasto-plastic self-consistent crystal plasticity and implicit finite elements: Applications to compression, cyclic tension-compression, and bending to large strains. Int. J. Plast. 93, 187-211.


SUMMARY AND FUTURE WORK

As already presented in the previous chapters, my dissertation is a result of an intensive and interdisciplinary research that cuts across fields of mechanics, materials science and applied mechanics. It is focused on the development of a novel material modeling techniques applied to elucidate mechanical response of metallic lamellar materials under complex loadings during their manufacturing. Moreover, deformation mechanism of twinning was investigated in detail. Deformation twins were represented as lamellar inclusions in the granular microstructures and overall the material behaved as a composite. The research approach that was chosen was based on crystal plasticity finite element modeling (CPFEM) framework, which is a full-field modeling technique. One of the main advantages of using this technique was that spatially resolved mechanical fields could be calculated within deformed microstructures. Hence, it was able to overcome the local stress state limitations which were present in the mean-field polycrystalline plasticity techniques, due to homogenization of each grain’s surroundings.

The developed techniques represent a very novel and unique modeling tool set which is able to provide significant insights into how different classes of metallic materials deform at various conditions. A two-level homogenization constitutive model for polycrystalline metals that deform by a combination of slip and twinning is presented in the chapter 1. An outstanding achievement is that the model was able to successfully capture the anisotropic material behavior of AZ31 across wide ranges of temperatures and strain rates using a single set of material parameters. The formulation of the developed model is sufficiently general, hence it can be easily applied to other materials that deform by slip and twin, which is, in my opinion, one of its greatest strengths. In the future work, this model can be used to investigate mechanical behavior of different materials, e.g. some different magnesium alloys, such as magnesium rare-earth alloy
WE43. As additional future work, this model, thanks to its capabilities, can be used to investigate and predict the fracture behavior of the polycrystalline materials.

In chapters 2, 3 and 4, the developed CPFE model is presented for two-phase polycrystalline HCP/BCC Zr/Nb layered composite, where hardening law was governed by the evolution of dislocation densities for multiple slip modes. In each of the above mentioned chapters a specific variation/formulation of the model was used. Overall, the developed model successfully predicted the stress-strain responses and texture evolution in both co-deforming phases in the composite to very large plastic strains. It also provided insights into the active slip systems that operate in both phases. Finite element granular microstructures were generated and initialized by the experimentally measured crystal orientations, grain shapes and grain sizes. This novel technique enabled analysis of microstructural heterogeneities during the rolling deformation of the composite. Furthermore, it unveiled the role of the microstructure and the annealing-induced changes in the microstructure in the development of the local strain concentrations (shear band formation) in the composite. Further steps that could be taken as a future work to potentially increase the capabilities of the developed model can consider implementation of a failure criterion in the constitutive relationships.

Chapter 5 describes developed CPFE model used to determine elastic and plastic behavior of Mg/Nb nano-layered composites. Micro-pillar composites were deformed in normal, parallel and 45 degree configuration and appropriate FE granular microstructures were generated. In order to determine the plastic response of the composites confined layer slip (CLS) model was successfully numerically implemented. In the future work, cohesive zone elements can be implemented in the model at the composite interphase. This would allow modeling of the interphacial sliding which was observed in 45 degree composite cases.
Chapters 6, 7 and 8 show three applications of a unique modeling technique that explicitly incorporates deformation twins into CPFE framework. This developed modeling technique models the morphological and crystallographic reorientation associated with the formation and thickening of a twin lamella in an explicit way using finite element homogenization scheme. This novel modeling approach was successfully applied to investigate twin formation in a cast uranium (chapter 6). Furthermore, the effects of dislocation densities in the twin domain were examined on twin formation and thickening. Simulations were carried out for \( \{\overline{1}012\}\langle10\overline{1}1\rangle \) extension twins in a magnesium alloy AZ31 where three types/cases of twin-dislocation density interactions were considered (chapter 7). One case assumes that the expanding twin retains in its domain the same dislocation density as the parent. The second one considers that twin expansion has lowered the dislocation density as the twin thickens, and the last one, the Basinski effect, assumes that when twin sweeps the region, the dislocation density incorporated in the twin domain is amplified (by two times). The last study (presented in chapter 8) examines formation of double twin structures in AZ31. Double twins have a great influence on material properties in general and they represent an important deformation mechanism. The predictions reveal a substantial activity of basal slip within the contraction portion of the double twin, causing strain localization in its vicinity. Finally, the simulations predict a gradient in the traction force field across twin-parent interface, suggesting that contraction twin-parent boundaries are weak links in the microstructure, where voids can nucleate. In the possible future work, this novel modeling approach can be used to further investigate the influence of twinning on the material response. One of the possible applications could be the investigation of the effects of twin-to-twin interactions on the specific material behavior.
APPENDIX

In order to explicitly incorporate a twin lamella into the finite element framework, a development of an automated procedure is required. This procedure was mentioned and discussed in more details in chapters 6, 7 and 8. A Matlab script has been developed, which writes Patran and Python script files containing specific commands for Patran and Abaqus, respectively. The Patran scripts are executed within Patran to perform either surface or solid meshing and the Python script files are executed within Abaqus to either extract the surface mesh from the solid mesh model or to perform the Abaqus mesh cleanup procedure. The final result of this procedure is a twin lamella of a desired volume inserted in a selected parent grain that maintains the overall conformity with the parent and neighboring grains. Codes are provided in the text below, that perform the most significant portion of this procedure. Furthermore, some useful comments are also provided.

% Matlab script: Extract_grains.m
% This script extracts all element sets - GRAINS from a part definition in the ABQ grain model
% Each element set (GRAIN) is then written as a separate ABQ input file (both node and element definitions)

clear all; clc;
% ----- INPUTS
% Define initial folder with FEA model file
init_folder = 'C:\Milan\PhD\Research\Mg_TWINSIMULATIONS\step6-6%_deformation2_DD';

% Define total number of grains in the model
num_grains = 35;

% Define name of the FEA input model
grain_file = 'AZ31_2_TWINS55%_DD_35.inp';

fid = fopen(strcat(init_folder,grain_file));

tline = fgetl(fid);
while(strcmp(tline,'*Node')==0)
tline = fgetl(fid);
end

% Read NODE coordinates
A = textscan(fid, '%u %f %f %f','delimiter',',','Whitespace','\n\r\t','MultipleDelimsAsOne',1);
nodeID = A{1}(:);
Xcoord = A{2}(:);
Ycoord = A{3}(:);
Zcoord = A{4}(:);

% Read ELEMENT connectivities
tline = fgetl(fid); % skip first line (e.g. *Element, type=C3D4)
A = textscan(fid, '%u %u %u %u','delimiter',',','Whitespace','\n\r\t','MultipleDelimsAsOne',1);

% Read ELEMENT SET definitions (GRAINS)
elements = cell(1,num_grains);
for i = 1:num_grains
    tline = fgetl(fid);  % skip line (e.g. *Elset, elset=GRAIN-0001, generate)
    A = textscan(fid, '%u %u %u', 'delimiter', ',', 'Whitespace', 'n\t', 'MultipleDelimsAsOne', 1);
    grainID = i;
    elements{i} = [A{1}(1):1:A{2}(1)]';
end
fclose(fid);

mkdir(strcat(init_folder, 'Meshed_Grains-INP'));

% Write ABQ input files for each element set
for i = 1:num_grains
    inp_addr = strcat(init_folder, 'Meshed_Grains-INP\Grain_', num2str(i), '.inp');
    z = 1;
    v = zeros(4*length(elements{i}), 4);
    f = zeros(length(elements{i}), 4);
    for j = 1:length(elements{i})
        v(z, 1) = node1(elements{i}(j)); v(z, 2) = Xcoord(node1(elements{i}(j)));
        v(z, 3) = Ycoord(node1(elements{i}(j))); v(z, 4) = Zcoord(node1(elements{i}(j)));
        v(z+1, 1) = node2(elements{i}(j)); v(z+1, 2) = Xcoord(node2(elements{i}(j)));
        v(z+1, 3) = Ycoord(node2(elements{i}(j))); v(z+1, 4) = Zcoord(node2(elements{i}(j)));
        v(z+2, 1) = node3(elements{i}(j)); v(z+2, 2) = Xcoord(node3(elements{i}(j)));
        v(z+2, 3) = Ycoord(node3(elements{i}(j))); v(z+2, 4) = Zcoord(node3(elements{i}(j)));
        v(z+3, 1) = node4(elements{i}(j)); v(z+3, 2) = Xcoord(node4(elements{i}(j)));
        v(z+3, 3) = Ycoord(node4(elements{i}(j))); v(z+3, 4) = Zcoord(node4(elements{i}(j)));
        z = z + 4;
        f(j, 1) = elements{i}(j);
        f(j, 2:5) = [node1(elements{i}(j)) node2(elements{i}(j)) node3(elements{i}(j))
                    node4(elements{i}(j))];
    end
    v = unique(v, 'rows');

% Write ABQ inp model
fprintf(fid2, '%d / %d\n', i, num_grains);
fid2 = fopen(inp_addr, 'w');
fprintf(fid2, '*HEADING\n');
fprintf(fid2, '*PART, name=PART-%i\n', i);
fprintf(fid2, '*NODE, NSET=ALL-%i\n', i);

% Write vertices (nodes)
for j = 1:length(v)
    fprintf(fid2, '%i, %g, %g, %g\n', v(j,1), v(j,2), v(j,3), v(j,4));
end

% Write faces (element connectivities)
for j = 1:length(f)
    fprintf(fid2, '%i, %g, %g, %g, %g\n', f(j,1), f(j,2), f(j,3), f(j,4), f(j,5));
end
fprintf(fid2, '*End Part\n');
fclose(fid2);
end
fprintf(1,'Complete\n');

% Matlab script: Python_script_TET2TRI.m
% This script writes Python script that converts meshed grains from solid mesh to surface mesh
% (shell or triangular elements)

clear all; clc;
%
% Define initial folder
init_folder = 'C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6\deformation2_DD\';
surface_mesh = strcat(init_folder,'GRAIN_Surface_mesh');
% Define total number of grains in the model
num_grains = 35;
python_name = strcat(init_folder,'TET2TRI.py');
mkdir(strcat(init_folder,'GRAIN_Surface_mesh'));

fid = fopen(python_name,'wt');
fprintf(fid,'# Python script - Solid to Surface mesh \n');
fprintf(fid,'from abaqus import *\n');
fprintf(fid,'from abaqusConstants import *\n');
fprintf(fid,'from part import *\n');
fprintf(fid,'from material import *\n');
fprintf(fid,'from section import *\n');
fprintf(fid,'from assembly import *\n');
fprintf(fid,'from step import *\n');
fprintf(fid,'from interaction import *\n');
fprintf(fid,'from load import *\n');
fprintf(fid,'from mesh import *\n');
fprintf(fid,'from job import *\n');
fprintf(fid,'from sketch import *\n');
fprintf(fid,'from visualization import *\n');
fprintf(fid,'from connectorBehavior import *\n');
fprintf(fid,'import regionToolset\n');
fprintf(fid,'import os\n');

%%
% Change working directory
%fprint(fid,'os.chdir("%s")\n',surface_mesh);
instance=";

for i = 1:num_grains
%fprint(fid,'#----------------------------------------\n');
inpname = strcat(['Grain_',num2str(i)]);
inp_addr = strcat(init_folder,'Meshed_Grains-INP\Grain_',num2str(i),'.inp');
%fprint(fid,'mdb.ModelFromInputFile(inputFileName="%s", name="%s")\n',inp_addr,inpname);
%fprint(fid,'grainModel%u = mdb.models["%s"]\n',i,inpname);  % model object
%fprint(fid,'part%u = grainModel%u.parts["PART-%u"]\n',i,i,i);  % part object
%fprint(fid,'nset%u = part%u.sets["ALL-%u"]\n',i,i,i);
%fprint(fid,'part%u.mergeNodes(nset%u)\n',i,i);
%fprint(fid,'part%u.convertSolidMeshToShell()\n',i);
%fprint(fid,'part%u.regenerate()\n',i);

fprintf(fid,'instance%u = grainModel%u.rootAssembly.Instance(name = "PART-1", part = part%u)
',i,i,i);
fprintf(fid,'job%u = mdb.Job(name="Grain_%u_surface_mesh", model = grainModel%u)
',i,i,i);
fprintf(fid,'job%u.writeInput()
',i);

fprintf(fid,'del mdb.models["%s"]
',inpname);
fprintf(fid,'del job%u
',i);

fprintf(fid,'Complete\n');

fprintf(fid,'*D elete model
fprintf(fid,'del mdb.models["%s"]
',inpname);
fprintf(fid,'del job%u
',i);
fprintf(fid,'\n');

eend

del mdb.models["%s"]

% Matlab script: createSTL.m
% This script creates STL files from deformed grain surface meshes. These STL files can be then
% meshed again (re-meshed), in order to avoid highly distorted elements
% (with overall bad aspect ratio)
clear all; clc;

% ----- INPUTS
% define folder with ABQ grain surface meshes
init_folder = 'C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6\deformation2_DD\';
% Define total number of grains in the model
num_grains = 35;
%
check = exist('STL_init','dir');
if (check ~= 7)
    mkdir(strcat(init_folder,'STL_init'));
end

for i = 1:num_grains
    file_name = strcat('Grain_',num2str(i),'_surface_mesh.inp');
    fid = fopen(strcat(init_folder,'GRAIN_Surface_mesh\',file_name));
    fprintf(fid,'%d / %d
',i,num_grains);
    tline = fgetl(fid);
    while strcmp(tline,'*Node')==0)
        tline = fgetl(fid);
    end
    A = textscan(fid,'%u %f %f %f','delimiter',',','Whitespace','\n\t','MultipleDelimsAsOne',1);
    nodeID = A{1}(:);
    new_nodeID = [1:1:length(A{1}(:))];
    NODEID = [nodeID new_nodeID];
    v(:,1) = A{2}(:);
    v(:,2) = A{3}(:);
    v(:,3) = A{4}(:);

    % Read ELEMENT connectivities
    tline = fgetl(fid);
    % skip line
    A = textscan(fid,'%u %u %u %u','delimiter',',','Whitespace','\n\t','MultipleDelimsAsOne',1);
    elementID = A{1}(:);
    f(:,1) = A{2}(:,1);
    f(:,2) = A{3}(:,1);
    f(:,3) = A{4}(:,1);
fclose(fid);

    for z = 1:length(f)
        for k = 1:3
            f(z,k) = NODEID(find(NODEID(:,1)==f(z,k),1),2);
        end
    end

% Define name for STL file
stl_name = strcat(init_folder,'STL_init\Grain_',num2str(i),'.stl');

FV = struct('vertices',v,'faces',f);
stlwrite(stl_name,FV,'mode','binary');
clear v; clear f;  % clear vertices and faces
end
fprintf(1,'Complete.\n');

% Matlab script: twin_inclusion.m
% This script forms a twin inclusion in a parent grain at the specific and pre-determined location.
clear all; clc;

% The path where the grain STLs are located
init_folder = 'C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6\%_deformation2_DD\';
% Define the parent grain
stl_name = 'Grain_1';
stladdr = strcat(init_folder,'data\\',stl_name,'.stl');

% Size of the edge subdivisions
seedsize = 1000;

% Define Patran database for meshing purposes
dbname = 'C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\TWIN_inclusion\2D.db';

% Two cell variables to store intersection points between cutting plane and
% the grain - used to reconstruct the twin "skin"
e_lr = cell(1,2); p_lr = cell(1,2); cut_pln = zeros(2,3);

% Open the Patran session file for writing  %if(side == 1)
    fid = fopen(strcat(init_folder,'\Patran_scripts\stl_to_2D_intersection.ses'),'wt');

% Variable declarations (needed for script to work properly)
fprintf(fid,'INTEGER i_segment_id\n');
fprintf(fid,'INTEGER i_number_of_groups\n');
fprintf(fid,'INTEGER fem_create_mesh_surfa_num_nodes\n');
fprintf(fid,'INTEGER fem_create_mesh_surfa_num elems\n');

fprintf(fid,'STRING crv_point1_list[VIRTUAL]\n');
fprintf(fid,'STRING crv_point2_list[VIRTUAL]\n');
fprintf(fid,'STRING pnt_output_ids[VIRTUAL]\n');
fprintf(fid,'STRING crv_output_ids[VIRTUAL]\n');
fprintf(fid,'STRING srf_output_ids[VIRTUAL]\n');
fprintf(fid,'STRING sa_group_list[32](1)\n');
fprintf(fid,'STRING s_target[6]\n');

We need to perform two cuts between the two cutting planes and the parent grain for
for t = 1:2
% Determine the side of the grain (cutting plane)
if(t == 1)
   side = 1; % left side
elseif(t == 2)
   side = 2; % right side
end

% Cutting plane normal
cut_pln_nrm = [0.5114, -0.4291, -0.7446];
% Normalization
cut_pln_nrm = cut_pln_nrm/norm(cut_pln_nrm,2);

% Cutting plane definition
% Define distance between the two cutting planes
distance = 4.75;
if(side == 1)
   % The coordinates of a point with the highest stress concentration
cut_pln_org = [61.3, 28, 55.1];
cut_pln(t,:) = cut_pln_org;
elseif(side == 2)
   % We have to translate cutting plane for a defined distance in the plane normal direction
cut_pln_org = cut_pln_org + distance*cut_pln_nrm/norm(cut_pln_nrm,2);
cut_pln(t,:) = cut_pln_org;
end

% Define cutting planes using three points,
% Plane equation: a(x-x0)+b(y-y0)+c(z-z0)=0 => new_point = (x,y,(-d-ax-by)/c)
pln = zeros(3,3);
pln(1,:) = cut_pln_org;
free_term = -dot3(cut_pln_nrm,cut_pln_org);
qq = find(cut_pln_nrm == 0);
if(size(qq,2) == 0)
   % We choose x and y and compute z coordinate of the point on the plane
   new_point = [1, 2, -(free_term + cut_pln_nrm(1,1)*1 + cut_pln_nrm(1,2)*2)/cut_pln_nrm(1,3)];
   pln(2,:) = new_point;
   new_point = [1, 5, -(free_term + cut_pln_nrm(1,1)*1 + cut_pln_nrm(1,2)*5)/cut_pln_nrm(1,3)];
   pln(3,:) = new_point;
elseif(size(qq,2) == 1)
   if((qq == 1) || (qq == 2))
      % We choose x and y and compute z coordinate of the point on the plane
      new_point = [1, 2, -(free_term + cut_pln_nrm(1,1)*1 + cut_pln_nrm(1,2)*2)/cut_pln_nrm(1,3)];
      pln(2,:) = new_point;
      new_point = [1, 5, -(free_term + cut_pln_nrm(1,1)*1 + cut_pln_nrm(1,2)*5)/cut_pln_nrm(1,3)];
      pln(3,:) = new_point;
   elseif(qq == 3)
      % We choose x and z and compute y coordinate of the point on the plane

   else
      % We choose y and z and compute x coordinate of the point on the plane
   end
end
new_point = [1, -(free_term + cut_pln_nrm(1,1)*1 + cut_pln_nrm(1,3)*2)/cut_pln_nrm(1,2),2];
pln(2,:) = new_point;
new_point = [1, -(free_term + cut_pln_nrm(1,1)*1 + cut_pln_nrm(1,3)*5)/cut_pln_nrm(1,2),5];
pln(3,:) = new_point;
end
elseif(size(qq,2) == 2)
qq = find(cut_pln_nrm ~= 0);
if(qq == 1) % y,z
pln(2,:) = [cut_pln_org(1,1) 10 20];
pln(3,:) = [cut_pln_org(1,1) 50 30];
elseif(qq == 2)
pln(2,:) = [10 cut_pln_org(1,2) 20];
pln(3,:) = [50 cut_pln_org(1,2) 20];
elseif(qq == 3)
pln(2,:) = [10 20 cut_pln_org(1,3)];
pln(3,:) = [50 20 cut_pln_org(1,3)];
end
elseif(size(qq,2) == 3)
warning('Plane vector normal is not correctly defined!!')
end

% Read the grain STL file
[v,f] = stlread(stladdr);
[v,f] = patchslim(v,f);

% The total number of faces and vertices in the STL file
numfaces = size(f,1);
umverts = size(v,1);

% Calculate face centers and face edge lengths
fc = zeros(numfaces,3);
fe = zeros(numfaces,3);
for i = 1:numfaces
v1 = v(f(i,1),:); v2 = v(f(i,2),:); v3 = v(f(i,3),:);
e1 = norm(v2-v1); e2 = norm(v3-v2); e3 = norm(v1-v3);
fci, = mean([v1;v2;v3],1);
fe(i,:) = [e1,e2,e3];
end

% Find max edge length in the mesh
maxe = max(max(fe));
globelemsize = round(0.7*maxe);

% Find all faces that are on the left side from the cutting plane (we have some faces that are cut)
if(side == 1) % left side
temp = 1;
for r = 1:size(fc,1)
[out,~] = determine_side(fc(r,:),cut_pln_nrm,cut_pln_org);
if(out==1)
tmp_left1(temp,1) = r;
temp = temp + 1;
end
end
elseif(side == 2) % right side
temp = 1; clear tmp_left1;
for r = 1:size(fc,1)
[out,~] = determine_side(fc(r,:),cut_pln_nrm,cut_pln_org);
if(out==2)
tmp_left1(temp,1) = r;
end
end

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temp = temp + 1;
end
end
end

% Remove faces that are cut
if (side == 2)
clear tmp_left;
end
kk = 1;
for z = 1:length(tmp_left1)
    index = tmp_left1(z);
    f1 = f(index,1); f2 = f(index,2); f3 = f(index,3);
    [c1,~] = determine_side(v(f1,:),cut_pln_nrm,cut_pln_org);
    [c2,~] = determine_side(v(f2,:),cut_pln_nrm,cut_pln_org);
    [c3,~] = determine_side(v(f3,:),cut_pln_nrm,cut_pln_org);
    if ((side == 1) && (c1+c2+c3 == 3) || (side == 2) && (c1+c2+c3 == 6))
        tmp_left(kk,1) = index;
        kk = kk+1;
    end
end
fl = f(tmp_left,:);
node_left = unique(fl);
v_left = v(node_left,:);
for g = 1:length(fl)
    for h = 1:3
        fl(g,h) = find(node_left == fl(g,h),1);
    end
end

index = 1;
if (side == 2)
clear tmp;
end
for z = 1:size(fc,1)
    [~,dist] = determine_side(fc(z,:),cut_pln_nrm,cut_pln_org);
    if (dist < maxe)
        tmp(index,1) = z;
        index = index + 1;
    end
end

% If the grain is being cut by the plane then cut it, if not, continue to the next grain
if ~isempty(tmp)
    % Remove all faces that are not cut
    fp = f(tmp,:); fc = fc(tmp,:); % f -> fp
    ind = [1,2;2,3;3,1];
    numfaces = size(fp,1);
    p = zeros(numfaces*2,3);
    e = zeros(numfaces,3); % Third column is for element/face ID that was cut
    l = -1;
    for i = 1:numfaces
        % Current face vertex coordinates (3x3 matrix of vertices)
        tri = round([v(fp(i,1,:)); v(fp(i,2,:)); v(fp(i,3,:))]*1e10)/1e10;
        % Check how many vertices are "to the right" of the plane. If 1 or 2 then the face is cut by the plane

sz1 = 0; sz2 = 0; mind2 = 0;
for z = 1:3
    [out,dist] = determine_side(tri(z,:),cut_pln_nrm,cut_pln_org);
    if(out == 2)
        sz1 = sz1 + 1;
    end
    if(dist == 0)
        sz2 = sz2 + 1;
        mind2 = z;
    end
end
% If the face is cut by the plane, continue, if not, jump to the next face
if(sz1 == 1 || sz1 == 2)
    % Find where (in local line coordinates) the plane intersects the edges of the triangle
    pen = triplapenchkwov(pln,tri);
    penind = find(pen>1e-16 & pen<1-1e-16);

    % Determine the points of the line segments (formed by triangle/cutting plane intersections).
    % These segments should form closed loops, which then can be meshed
    switch sz2
        case 0
            % If no vertices lie on the cutting plane, calculate the triangle/plane intersection points
            v11 = tri(ind(penind(1),1,:)); v12 = tri(ind(penind(1),2,:));
            v21 = tri(ind(penind(2),1,:)); v22 = tri(ind(penind(2),2,:));
        case 1
            % If one vertex lies on the plane and cutting plane intersects the triangle, one point of the
            % line segment is going to have the same coordinate as the vertex on the plane. The second point
            % coordinate is calculated as triangle/plane intersection
            if ~isempty(penind)
                p1 = tri(mind2(1,:),:);
                v11 = tri(ind(penind(1),1,:)); v12 = tri(ind(penind(1),2,:));
                t1 = pen(penind(1));
                p2 = v11+t1*(v12-v11);
            end
        case 2
            % If two vertices lie on the plane, both are written down as line segment points
            p1 = tri(mind2(1,:),:);
            p2 = tri(mind2(2,:),:);
    end
    l = l+2; % counter

    % Save the points into a matrix
    p(l,:) = p1; p(l+1,:) = p2;

    % The connectivity table
    e(ceil(l/2,:)) = [l,l+1,tmp(i)];
else
    % In this case, no points are saved, skip to the next grain
    warning(strcat('Problem. There are triangles lying on the cutting plane. Cannot produce a
section.Grain number: '),num2str(g));
end
% Remove duplicated vertices - resize
index = find(ismember(p,[0 0 0],'rows') == 1,1);
p = p(1:index-1,:);
index = find(e(:,1) == 0,1);
e = e(1:index-1,:);

% Remove duplicated nodes. Still we'll have some duplicated nodes due to rounding errors
[p, ~, indexn] = unique(p, 'rows');

maxx = max(max(e(:,1:2))); ee = zeros(size(e,1),3);
for z = 1:maxx
    [row,col] = find(e(:,1:2) == z);
    ee(row,col) = indexn(z); ee(row,3) = e(row,3);
end

% Find additional duplicated nodes (points) that are really close, but because of small numerical
% (round-off) error, they are perceived as different nodes; NOTE: p is sorted
for z = 1:length(p)-1
    if(abs(p(z,1)-p(z+1,1))<1e-6 & abs(p(z,2)-p(z+1,2))<1e-6 & abs(p(z,3)-p(z+1,3))<1e-6)
        p(z,:) = p(z+1,:);
    end
end

[p, indexm, indexn] = unique(p, 'rows'); % Remove duplicated points
for z = 1:max(max(ee(:,1:2)))
    [row,col] = find(ee(:,1:2) == z);
    for j = 1:length(row)
        e(row(j),col(j)) = indexn(z); e(row(j),3) = ee(row(j),3);
    end
end

% In this part, we have to save quantities p & e for left and right side of
% the grain in order to reconstruct twin "skin" (shell)
e_lr{1,t} = e;
p_lr{1,t} = p;

% We need to append these cut elements (to the left or right side of grain)
nodemax = max(max(fl));
e_append = e(:,1:2) + nodemax;
if(side == 1) % left side
    elmnt_left = size(fl,1);
elseif(side == 2) % right side
    elmnt_right = size(fl,1);
end
for z = 1:size(e,1) % The number of intersected elements
    nds = zeros(1,2);
    xx = zeros(1,5); yy = zeros(1,5); zz = zeros(1,5);
    gelem = e(z,3); elmnt = length(fl);
    nodes = [fl(gelem,1) fl(gelem,2) fl(gelem,3)];
    % Determine which nodes are important (on which side of the cutting plane they are)
    kk = 1;
    for j = 1:3
        [out,~] = determine_side(v(nodes(1,j),:),cut_pln_nrm,cut_pln_org);
        if((out == 1) & (side == 1)) % Nodes that we need
            nds(kk) = nodes(1,j);
            kk = kk +1;
        elseif((out == 2) & (side == 2)) % Nodes that we need
            nds(kk) = nodes(1,j);
            kk = kk +1;
    end
end
% Generate new elements (connect part of the grain with the intersected plane)
if(isempty(find(nds == 0,1) == 1) && (length(unique(nds)) == 2)) % you have two nodes
    sznds = 2;
    cc = setdiff(nodes, nds);
else
    sznds = 1;
end
if(sznds == 1) % We have one node
    ff1 = find(ismember(v_left, v(nds(1,1),:),'rows') == 1,1);
    fl(elmnt+1,:) = [e_append(z,1) e_append(z,2)];
elseif(sznds == 2) % We have two nodes
% Finding intersections between lines - NOTE: You will always have an
% intersection, because all these nodes lie on the same plane. This is the
% plane of the element (these 5 points are coplanar points)
% point1  point2  point3  point4  point5 (node that is cut, it's on the right side)
    xx = [p(e(z,1),1) p(e(z,2),1) v(nds(1,1),1) v(nds(1,2),1) v(cc,1)];
    yy = [p(e(z,1),2) p(e(z,2),2) v(nds(1,1),2) v(nds(1,2),2) v(cc,2)];
    zz = [p(e(z,1),3) p(e(z,2),3) v(nds(1,1),3) v(nds(1,2),3) v(cc,3)];

% take points 1,3,5
    vector1 = [xx(1)-xx(5) yy(1)-yy(5) zz(1)-zz(5)]; % 1-5
    vector2 = [xx(3)-xx(5) yy(3)-yy(5) zz(3)-zz(5)]; % 3-5
    vcross = cross3(vector1,vector2);
    ff1 = find(ismember(v_left, v(nds(1,1),:),'rows') == 1,1);
    ff2 = find(ismember(v_left, v(nds(1,2),:),'rows') == 1,1);

if(norm(vcross,2) <= 1e-6) % This means that nodes 1,3,5 are co-linear -> elements 124 & 134
    fl(elmnt+1,:) = [e_append(z,1) e_append(z,2) ff2];
    fl(elmnt+2,:) = [e_append(z,1) ff1 ff2];
else % This means that nodes 2,3,5 are co-linear -> elements 123 & 134
    fl(elmnt+1,:) = [e_append(z,1) e_append(z,2) ff1];
    fl(elmnt+2,:) = [e_append(z,1) ff1 ff2];
end
end
end

% Append the vertices (intersection nodes between the cutting plane and the grain mesh)
v_left = [v_left;p];
if(side == 1)
    stlwrite(strcat(init_folder, 'STLs\', stl_name, '_Left_part.stl'), fl, v_left);
    fprintf(1, '1. Left part of the grain is done.\n');
    % Select elements that are added to append them to ring file - left side
    f_ringl = fl(elmnt_left+1:end,:);
    v_ringl = v_left;
    [v_ringl,f_ringl] = patchslim(v_ringl,f_ringl);
else % This means that nodes 2,3,5 are co-linear -> elements 123 & 134
    stlwrite(strcat(init_folder, 'STLs\', stl_name, '_Right_part.stl'), fl, v_left);
    fprintf(1, '2. Right part of the grain is done.\n');
    % Select elements that are added to append them to ring file - right side
    f_ringr = fl(elmnt_right+1:end,:);
    v_ringr = v_left;
    [v_ringr,f_ringr] = patchslim(v_ringr,f_ringr);
end
% Write Patran session file to perform meshing
% If every loop is closed, write Patran commands for the current grain
noloop = 0;
if noloop == 0;

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% Go through every loop in the grain section. NOTE: I renamed el into e
for i = 1:1 %size(e,2)-1
    numedges = size(e,1);

    % Form the matrix of the line segment points. j=1 staring points, j=2 ending points
    for j = 1:2
        fprintf(fid,'crv_point%s_list = "@\n',num2str(j));
        for k = 1:numedges
            fprintf(fid,[' %.6f %.6f %.6f '],p(e(k,j),:));
            if k<numedges
                fprintf(fid,'@
');
            else
                fprintf(fid,'"
');
            end
        end
    end

    % Draw line segments
    fprintf(fid,'asm_const_line_2point( ", crv_point1_list, @\n crv_point2_list, 0 "", 50., 1, crv_output_ids )
    fprintf(fid,'sgm_create_curve_chain_v1( ", crv_output_ids, @\n TRUE, i_segment_id, @\n crv_output_ids )
    fprintf(fid, '"? YES 38000217"
    fprintf(fid,'sgm_create_surface_trimmed_v1( "1", crv_output_ids,"", ", TRUE, TRUE, TRUE, 
TRUE,@\n srf_output_ids )
    fprintf(fid,'mesh_seed_display_mgr.erase( )
    fprintf(fid,'mesh_seed_create( "Surface"
    for k = 1:numedges
        tmp = strcat(' 1.' ,num2str(k));
        fprintf(fid,'%s',tmp);
        if mod(k,10) == 0
            fprintf(fid,'@
');
        end
    end
    fprintf(fid, '"", 2, 0., %u., 0. )
    meshsize);

    % Mesh the surface (uses global element size defined at the beginning)
    fprintf(fid,'fem_create_mesh_surf_4( "Hybrid", 49680, "Surface 1", @\n 4, ["%f", "0.1", "0.2", 
"1.0"], "Tria3", @\n"
    fem_create_mesh_surf_num_nodes, fem_create_mesh_surf_num_elements, fem_create_mesh_s_nodes_created, @\n    fem_create_mesh_s_elements_created )
    fprintf(fid,'list_create_curve_ass_group ( sa_group_list, i_number_of_groups, s_target, @\n    crv_output_ids ) );
    fprintf(fid,'asm_delete_curve( crv_output_ids,asm_delete_any_deleted_ids )
    fprintf(fid,'asm_delete_curve( crv_output_ids,asm_delete_any_deleted_ids )

    % Find and store IDs of all points in the model, and finally delete them
    fprintf(fid, 382}
fprintf(fid, 'list_create_point_ass_group % ( sa_group_list, i_number_of_groups, s_target, %
pt_output_ids )
');
fprintf(fid, 'asm_delete_point( pt_output_ids, asm_delete_any_deleted_ids )
');

% Find and store IDs of all surfaces in the model, and finally delete them
fprintf(fid, 'list_create_surface_ass_group % ( sa_group_list, i_number_of_groups, s_target, %
srf_output_ids )
');
fprintf(fid, 'asm_delete_surface( srf_output_ids, asm_delete_any_deleted_ids )
');

end
% Generate the file name of the mesh export file
if (side == 1)
    neuexportname = strcat(init_folder, 'data\', stl_name, '_left.out');
else (side == 2)
    neuexportname = strcat(init_folder, 'data\', stl_name, '_right.out');
end
% Export
fprintf(fid, 'neutral_export2( "%s", "P3/PATRAN Neutral File from: %s", [TRUE, TRUE, FALSE, FALSE, %
FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE], TRUE, 1, [0] )
');
% Find and store IDs of all FEA elements in the model, delete them and associated nodes
fprintf(fid, 'list_create_elem_ass_group % ( 0, sa_group_list, i_number_of_groups, s_target, %
fem_create_mesh_s_elems_created )
');
fprintf(fid, 'fem_delete_elem_and_node(fem_create_mesh_s_elems_created,sv_deleted_elements)
');
end
clear e p;
end % End of t
fclose(fid);

fprintf(1, '3. Processing twin part...
');
% Reconstruct the twin "skin"
% Read the grain STL file
[v,f] = stlread(stladdr);
[v,f] = patchslim(v,f);
numfaces = size(f,1);
% Calculate face centers for all faces (elements)
fc = zeros(numfaces,3);
for i = 1:numfaces
    v1 = v(f(i,1,:),:); v2 = v(f(i,2,:),:); v3 = v(f(i,3,:),:);
    fc(i,:) = mean([v1;v2;v3],1);
end
% Find all faces that are potentially between the two cutting planes (inside the twin "skin")
index = 1;
for z = 1:size(fc,1)
    [out1,~] = determine_side(fc(z,:),cut_pln_nrm,cut_pln(1,:));
    [out2,~] = determine_side(fc(z,:),cut_pln_nrm,cut_pln(2,:));
    if ((out1 == 2) && (out2 == 1))
        tmp_twin1(index,1) = z;
        index = index + 1;
    end
end
Here we make a small addition - in some really rare occasions, it can happen that the element center is not between the two cutting planes, even though it is being cut. For that reason we will add all elements to tmp_twin1 that have being cut.

```matlab
tmp = [e_lr{1,1}{(:,3)}; e_lr{1,2}{(:,3)}];
tmp = unique(tmp);
tmp_twin1 = [tmp_twin1;tmp];

tmp_twin = [];
% Remove those faces that are cut
if(isempty(tmp_twin1) == 0) %Maybe we don't have elements between cutting planes;
    kk = 1;
    for z = 1:length(tmp_twin1)
        index = tmp_twin1(z);
        f1 = f(index,1); f2 = f(index,2); f3 = f(index,3);
        [out1,~] = determine_side(v(f1,:),cut_pln_nrm,cut_pln(1,:));
        [out2,~] = determine_side(v(f2,:),cut_pln_nrm,cut_pln(1,:));
        [out3,~] = determine_side(v(f3,:),cut_pln_nrm,cut_pln(1,:));
        [out4,~] = determine_side(v(f1,:),cut_pln_nrm,cut_pln(2,:));
        [out5,~] = determine_side(v(f2,:),cut_pln_nrm,cut_pln(2,:));
        [out6,~] = determine_side(v(f3,:),cut_pln_nrm,cut_pln(2,:));
        if((out1+out2+out3 == 6) && (out4+out5+out6 == 3))
            tmp_twin(kk,1) = index;
            kk = kk+1;
        end
    end
end
% Select faces between the two cutting planes - elements that are entirely between the planes
if(isempty(tmp_twin) == 0)
    ftw = f(tmp_twin,,:);
    node_twin = unique(ftw);
    v_twin = v(node_twin,:);
    for g = 1:size(ftw,1)
        for h = 1:3
            ftw(g,h) = find(node_twin == ftw(g,h),1);
        end
    end
else % This is the case when we don't have entire elements (faces) in the twin
    ftw = zeros(0,3);
    v_twin = zeros(0,3);
end
% NOTE: v_twin also includes nodes that are in the twin (elements made of these nodes are cut - if the twin is small)
index1 = size(v_twin,1);
for z = 1:length(tmp_twin1)
    index = tmp_twin1(z);
    fff = [f(index,1) f(index,2) f(index,3)];
    for d = 1:3
        [out1,~] = determine_side(v(fff(d,:),cut_pln_nrm,cut_pln(1,:)));
        [out2,~] = determine_side(v(fff(d,:),cut_pln_nrm,cut_pln(2,:)));
        if((out1 == 2) && (out2 == 1))
            index1 = index1 + 1;
            v_twin(index1,:) = v(fff(d,:));
        end
    end
end
end
```
[v_twin,ftw] = patchslim(v_twin,ftw);
% Find the biggest nodeID
nodemax = size(v_twin,1);

% Append elements that have been cut
% Really important note - there are some elements that are cut with both planes - we consider them
% at the end. These elements can be found in both right and left side of the cut - e_lr
nodes = zeros(1,3); elmnt = size(ftw,1); kkk=1; spec_elm = [];
for s = 1:2 % Two passes, one for each side (left and right)
    if(s == 1)
        e_append = e_lr{1,s}(1:2) + nodemax;
        nodemax_left = nodemax;
    else
        nodemax_right = max(max(e_append));
        e_append = e_lr{1,s}(1:2) + max(max(e_append));
    end
    for z = 1:length(e_lr{1,s})
        nds = zeros(1,2);
        xx = zeros(1,5); yy = zeros(1,5); zz = zeros(1,5);
        gelem = e_lr{1,s}(z,3); elmnt = size(ftw,1);
        nodes = [f(gelem,1) f(gelem,2) f(gelem,3)];
        % Determine which nodes are important (on which side of the cutting plane are they)
        kk = 1;
        for j = 1:3
            [out1,~] = determine_side(v(nodes(1,j),:),cut_pln_nrm,cut_pln(1,:));
            [out2,~] = determine_side(v(nodes(1,j),:),cut_pln_nrm,cut_pln(2,:));
            if((out1 == 2) && (s == 1)) % Nodes that we need, left side
                nds(kk) = nodes(1,j);
                kk = kk +1;
            elseif((out2 == 1) && (s == 2)) % Nodes that we need, right side
                nds(kk) = nodes(1,j);
                kk = kk +1;
            end
        end
        % Generate new elements (connect part of the grain with the intersected plane)
        if(isempty(find(nds == 0,1) == 1) && (length(unique(nds))==2)) % you have two nodes
            sznds = 2;
            cc = setdiff(nodes,nds);
        else
            sznds = 1;
        end
        if(sznds == 1) % We have one node
            ff1 = find(ismember(v_twin,v(nds(1,1,:),)'rows') == 1,1);
            if(isempty(ff1) == 1)
                spec_elm(kkk,1) = gelem;
                kkk = kkk +1;
                continue
            end
            ftw(elmnt+1,:) = [ff1 e_append(z,1) e_append(z,2)];
        elseif(sznds == 2) % We have two nodes
            % Finding intersections between line - NOTE: You will always have an
            % intersection because all these nodes lie in the plane of the elements
            % point1  point2  point3  point4  point5
            xx = [p_lr{1,s}(e_lr{1,s}(z,1),1) p_lr{1,s}(e_lr{1,s}(z,2),1) v(nds(1,1),1) v(nds(1,2),1) v(cc,1)];
            yy = [p_lr{1,s}(e_lr{1,s}(z,1),2) p_lr{1,s}(e_lr{1,s}(z,2),2) v(nds(1,1),2) v(nds(1,2),2) v(cc,2)];
            zz = [p_lr{1,s}(e_lr{1,s}(z,1),3) p_lr{1,s}(e_lr{1,s}(z,2),3) v(nds(1,1),3) v(nds(1,2),3) v(cc,3)];
% Determine connectivities between the nodes
% Take points 1,3,5
vector1 = [xx(1)-xx(5) yy(1)-yy(5) zz(1)-zz(5)]; % 1-5
vector2 = [xx(3)-xx(5) yy(3)-yy(5) zz(3)-zz(5)]; % 3-5
vcross = cross3(vector1,vector2);

ff1 = find(ismember(v_twin,v(nds(1,1),:),'rows') == 1,1);
ff2 = find(ismember(v_twin,v(nds(1,2),:),'rows') == 1,1);
if(isempty(ff1) == 1 || isempty(ff2) == 1)
    spec_elm(kkk,1) = gelem;
    kkk = kkk + 1;
    continue
end
if(norm(vcross,2) <= 1e-6) % This means that nodes 1,3,5 are co-linear -> elements 124 & 134
    ftw(elmnt+1,:) = [e_append(z,1) e_append(z,2) ff2];
    ftw(elmnt+2,:) = [e_append(z,1) ff1 ff2];
else % This means that nodes 2,3,5 are co-linear -> elements 123 & 134
    ftw(elmnt+1,:) = [e_append(z,1) e_append(z,2) ff1];
    ftw(elmnt+2,:) = [e_append(z,1) ff1 ff2];
end
end

% Append vertices (intersection nodes between the cutting plane and the grain mesh)
v_twin = [v_twin;p_lr{1,s}];
end

% Now we deal with the elements that are cut in two different places - these elements are in array
% spec_elm
if(isempty(spec_elm) ~= 0)
    spec_elm = unique(spec_elm);
    for i = 1:size(spec_elm,1)
        elmnt = size(ftw,1); innode = [];
        % We consider each element separately
        gelem = spec_elm(i,1);
        % Element vertices
        Tnodes = [f(gelem,1) f(gelem,2) f(gelem,3)];
        % Element intersection points
        ind1 = find(e_lr{1,1}(:,3) == gelem); % left side
        ind2 = find(e_lr{1,2}(:,3) == gelem); % right side
        % We relate intersection nodes to v_twin
        cut_nodes = [e_lr{1,1}(ind1,1:2)+nodemax_left e_lr{1,2}(ind2,1:2)+nodemax_right];
        % We check which node is between the cutting twin planes
        for j = 1:3
            [out1,~] = determine_side(v(Tnodes(1,j),:),cut_pln_nrm,cut_pln(1,:));
            [out2,~] = determine_side(v(Tnodes(1,j),:),cut_pln_nrm,cut_pln(2,:));
            if((out1 == 2) && (out2 == 1))
                innode = j;
            end
        end
        sequence = [];
        if(isempty(innode) == 1) % No vertices between the cutting planes
            for j = 1:4 % T1-T3 edge
                vector1 = [v(Tnodes(1,j),1)-v(Tnodes(1,1),1) v(Tnodes(1,3),2)-v(Tnodes(1,1),2)
                            v(Tnodes(1,3),3)-v(Tnodes(1,1),3)];
                vector2 = [v_twin(cut_nodes(1,j),1)-v(Tnodes(1,1),1) v_twin(cut_nodes(1,j),2)-v(Tnodes(1,1),2)
                            v_twin(cut_nodes(1,j),3)-v(Tnodes(1,1),3)];
                vcross = cross3(vector1,vector2);
            end
        end
end

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if(vcross <= 1e-6) % This intersection point is co-linear with the other two nodes
    sequence = [sequence j];
end
end

for j = 1:4 % T1-T2 edge
    vector1 = [v(Tnodes(1,2),1)-v(Tnodes(1,1),1) v(Tnodes(1,2),2)-v(Tnodes(1,1),2)
      v(Tnodes(1,2),3)-v(Tnodes(1,1),3)];
    vector2 = [v_twin(cut_nodes(1,j),1)-v(Tnodes(1,1),1) v_twin(cut_nodes(1,j),2)-v(Tnodes(1,1),2)
      v_twin(cut_nodes(1,j),3)-v(Tnodes(1,1),3)];
    vcross = cross3(vector1,vector2);
    if(vcross <= 1e-6) % This intersection point is co-linear with the two nodes
        sequence = [sequence j];
    end
end

if(size(sequence,2) < 4)
    for j = 1:4 % T2-T3 edge
        vector1 = [v(Tnodes(1,3),1)-v(Tnodes(1,2),1) v(Tnodes(1,3),2)-v(Tnodes(1,2),2)
          v(Tnodes(1,3),3)-v(Tnodes(1,2),3)];
        vector2 = [v_twin(cut_nodes(1,j),1)-v(Tnodes(1,2),1) v_twin(cut_nodes(1,j),2)-v(Tnodes(1,2),2)
          v_twin(cut_nodes(1,j),3)-v(Tnodes(1,2),3)];
        vcross = cross3(vector1,vector2);
        if(vcross <= 1e-6) % This intersection point is co-linear with the two nodes
            sequence = [sequence j];
        end
    end
end
end

% Now, we create new elements
ftw(elmnt+1,:) = [cut_nodes(1,sequence(1,1)) cut_nodes(1,sequence(1,3))
    cut_nodes(1,sequence(1,4))];
ftw(elmnt+2,:) = [cut_nodes(1,sequence(1,1)) cut_nodes(1,sequence(1,2))
    cut_nodes(1,sequence(1,4))];
elseif(size(innode,1)==1) % One element vertex between the two nodes
    if(innode == 1)
        j1 = 2; j2 = 3;
    elseif(innode == 2)
        j1 = 1; j2 = 3;
    elseif(innode == 3)
        j1 = 1; j2 = 2;
    end
    sequence = [];
    for j = 1:4
        vector1 = [v(Tnodes(1,innode),1)-v(Tnodes(1,j1),1) v(Tnodes(1,innode),2)-v(Tnodes(1,j1),2)
          v(Tnodes(1,innode),3)-v(Tnodes(1,j1),3)];
        vector2 = [v_twin(cut_nodes(1,j),1)-v(Tnodes(1,j1),1) v_twin(cut_nodes(1,j),2)-v(Tnodes(1,j1),2)
          v_twin(cut_nodes(1,j),3)-v(Tnodes(1,j1),3)];
        vcross = cross3(vector1,vector2);
        if(vcross <= 1e-6) % This intersection point is co-linear with the two nodes
            sequence = [sequence j];
            break;
        end
    end
end
for j = 1:4
    vector1 = [v(Tnodes(1,innode),1)-v(Tnodes(1,j2),1) v(Tnodes(1,innode),2)-v(Tnodes(1,j2),2)
      v(Tnodes(1,innode),3)-v(Tnodes(1,j2),3)];
    vector2 = [v_twin(cut_nodes(1,j),1)-v(Tnodes(1,j2),1) v_twin(cut_nodes(1,j),2)-v(Tnodes(1,j2),2)
      v_twin(cut_nodes(1,j),3)-v(Tnodes(1,j2),3)];
vcross = cross3(vector1, vector2);
if (vcross <= 1e-6)  % This intersection point is co-linear with the two nodes
sequence = [sequence j];
    break;
end
end

switch(sequence(1,1))
    case 1
        sequence(1,3) = 2;
    case 2
        sequence(1,3) = 1;
    case 3
        sequence(1,3) = 4;
    case 4
        sequence(1,3) = 3;
end

switch(sequence(1,2))
    case 1
        sequence(1,4) = 2;
    case 2
        sequence(1,4) = 1;
    case 3
        sequence(1,4) = 4;
    case 4
        sequence(1,4) = 3;
end

ff1 = find(ismember(v_twin, v(Tnodes(1, innode), :), 'rows') == 1, 1);
% Create new elements - 3 elements
ftw(elmnt+1,:) = [cut_nodes(1, sequence(1,1)) cut_nodes(1, sequence(1,2)) ff1];
ftw(elmnt+2,:) = [cut_nodes(1, sequence(1,1)) cut_nodes(1, sequence(1,3)) cut_nodes(1, sequence(1,4))];
ftw(elmnt+3,:) = [cut_nodes(1, sequence(1,1)) cut_nodes(1, sequence(1,2)) cut_nodes(1, sequence(1,4))];
end
end
end

% Write STL file of the twin region or "skin"
stlwrite(strcat(init_folder, 'STLs\', stl_name, '_Twin.stl'), ftw, v_twin);

% Now, we write the twin grain ring file
elmnt = size(ftw,1);
nodemax = max(max(ftw));
% The left part
vring = [v_twin; v_ringl];
fring = [ftw; f_ringl+nodemax];
% The right part
nodemax = max(max(fring));
vring = [vring; v_ringr];
fring = [fring; f_ringr+nodemax];

% Write STL file of the twin grain ring
stlwrite(strcat(init_folder, 'STLs\', stl_name, '_RING.stl'), fring, vring);

fprintf(1, 'Complete
');
% Matlab function: determine_side.m
% This function determines if the point is on the left or right side of the plane in 3D space.
% function [out,distance] = determine_side(point,normal,point_plane)
% We take point and normal vector to define line
% Line equation as a function of parameter t (parametric form)
x = @(t) normal(1,1)*t + point(1,1);
y = @(t) normal(1,2)*t + point(1,2);
z = @(t) normal(1,3)*t + point(1,3);

% We are trying to solve plane equation - find parameter t
plane = @(t) normal(1,1)*(x(t) - point_plane(1,1))+normal(1,2)*(y(t) - point_plane(1,2))+normal(1,3)*(z(t) - point_plane(1,3));
t = fzero(plane,0);

% Projection of the point onto the plane
proj = [x(t) y(t) z(t)];
vector = point - proj;
distance = norm(vector,2);

% We compute dot product between the vector and normal plane vector (they are colinear), but the
% side on which the point is will depend on the sign of the dot(scalar) product.
temp = vector(1,1)*normal(1,1) + vector(1,2)*normal(1,2) + vector(1,3)*normal(1,3);
if(temp > 0)
    out = 2; % Right side
else
    out = 1; % Left side
end
end

% This script is processing Patran output files (meshed intersection 2D planes – which we got as
% intersections between the parent grain and two twin cutting planes).
% As a result, we create two STL files for each intersection plane (left and right side).

clear all; clc;

% Where the .out files are (meshed grains)
init_folder = 'C:\Milan\PhD\Research\Mg_TWINSIMULATIONS\step6-6\%deformation2_DD\data\';
init_fname = 'Grain_';
neu_ext = '.out';

% Total number of grains in the model
numall = 34;
% Counter
k = 0;
% Memory allocation
numnodes = zeros(1,numall);
umelems = zeros(1,numall);
coortable = cell(1,numall);
contable = cell(1,numall);

% Go through all the grains
for i = 1:numall
    % Progress output
    fprintf(1,'%d / %d\n',i,numall);
    for gg = 1:2 % Left and right side
        % Generate the filenames of the two intersection planes
if (gg == 1)
    outname = strcat(init_fname,num2str(i),'_left');
elseif (gg == 2)
    outname = strcat(init_fname,num2str(i),'_right');
end
outaddr = strcat(init_folder,outname,neu_ext);

% Open file, if no such file, move to the next one
fid = fopen(outaddr);
if fid ~= -1
    k = k+1;
    textscan(fid,'%s',2,'delimiter','\n'); % Skip lines

    % Read and store the number of elements/faces in the file
    A = textscan(fid,'%*d %*d %*d %*d %u %u %*[\n]'1,'\n\t','\n\t','\n\t','\n\t','\n\t','\n\t',1); % Ignore whitespace
    numnodes(k) = A{1}(:);
    numelemsi = A{2}(:);
    textscan(fid,'%s',1,'delimiter','\n'); % Skip a line

% Memory allocation
coortable{k} = zeros(numnodes(k),3);
contable{k} = zeros(numelemsi,3);

% ADD CHECK FOR START OF NODE OUTPUT IF NECESSARY

% Read all node coordinates
for j = 1:numnodes(k)
    textscan(fid,'%s',1,'delimiter','\n'); % Skip line
    A = textscan(fid,'%f %f %f',1,'\b','\b','\b','\n\t','\n\t',1); % Read node coordinates
    coortable{k}(j,1:3) = [A{1}(:),A{2}(:),A{3}(:)];
    textscan(fid,'%s',1,'delimiter','\n'); % Skip a line
end

% ADD CHECK FOR START OF ELEMENT OUTPUT IF NECESSARY

% Read the element connectivity table
m = 1;
for j = 1:numelemsi
    A = textscan(fid,'%u %u %u %*[\n]'1,'\b','\b','\b',1); % Read element connectivity
    elmtype = A{2}(:);
    if elmtype == 3
        textscan(fid,'%s',1,'delimiter','\n'); % Skip lines
        A = textscan(fid,'%u %u %u',1,'\b','\b',1); % Read triangular element coordinates
        contable{k}(m,:) = [A{1}(:),A{2}(:),A{3}(:)];
        % Triangular element area calculation
        node1i = coortable{k}(contable{k}(m,1,:));
        node2i = coortable{k}(contable{k}(m,2,:));
        node3i = coortable{k}(contable{k}(m,3,:));
        v1i = node1i-node2i;
        v2i = node1i-node3i;
        m = m+1;
    else
    end
    textscan(fid,'%s',2,'delimiter','\n'); % Skip lines
end

% Clean up
contable{k}(contable{k}(;,1)==0,:) = [];
contable{k}(;,4) = i;
numelems(k) = size(contable{k},1);
v = coortable{k};
f = contable{k}(;,1:3);

fclose(fid);
if (gg == 1)
stlwrite(strcat('C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6\%_deformation2_DD\STLs\',init_fname,num2str(i),'_left_plane.stl'),f,v);
elseif (gg == 2)
stlwrite(strcat('C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6\%_deformation2_DD\STLs\',init_fname,num2str(i),'_right_plane.stl'),f,v);
end
% Delete Patran output file
delete(strcat(init_folder,outname,neu_ext));
else
v = [-1000,-1000,-1000; -1001, -1001, -1001; -1000,-1001,-1001];
f = [1,2,3];
end
end
end

fprintf(1,'Complete.n');

% This script merges STL files in order to get parent and twin grain. We merge two intersection planes
% with the rest of the grain's parts.
clear all; clc;
grainID = 1;
init_folder = 'C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6\%_deformation2_DD\STLs\';

% Load left side of the grain
[v1,f1] = stlread(strcat(init_folder,'Grain_',num2str(grainID),'_Left_part.stl'));
% Load left intersection plane
[v2,f2] = stlread(strcat(init_folder,'Grain_\',num2str(grainID),'_left_plane.stl'));
v_left = [v1;v2];
f_left = [f1;f2];

% Process right side of the grain and right intersection plane
[v3,f3] = stlread(strcat(init_folder,'Grain_\',num2str(grainID),'_Right_part.stl'));
[v4,f4] = stlread(strcat(init_folder,'Grain_\',num2str(grainID),'_right_plane.stl'));
v_right = [v3;v4];
f_right = [f3;f4];
v_grain = [v_left;v_right];
f_right = f_right + length(v_left);
f_grain = [f_left,f_right];

% Write STL file
stlwrite(strcat(init_folder,'PARENT_GRAIN.stl'),f_grain,v_grain,'mode','binary');

% Merge STL file to form a twin
```matlab
[v5,f5] = stlread(strcat(init_folder,'Grain_',num2str(grainID),'_Twin.stl'));
[v6,f6] = stlread(strcat(init_folder,'Grain_',num2str(grainID),'_left_plane.stl'));
[v7,f7] = stlread(strcat(init_folder,'Grain_',num2str(grainID),'_right_plane.stl'));
v_twin = [v5;v6;v7];
f6 = f6 + length(v5);
f7 = f7 + length(v5) + length(v6);
f_twin = [f5;f6;f7];

% write STL
stlwrite(strcat(init_folder,'TWIN.stl'),f_twin,v_twin,'mode','binary');

fprintf(1,'Complete.
'); % The end

%% Matlab script: mesh_twin_neighbor.m
% This script mirrors "twin nodes" to all neighboring grains that are affected with twin inclusion.
% NOTE: intersection nodes have to be added to all neighboring grains so that we have conformal
% mesh from each side of the twin grain.
% GrainID is the ID of the twinned grain - Parent grain

clear all; clc;

% Define the initial folder
init_folder = 'C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6\%_deformation2_DD\';
% ID of the parent grain
grainID = 1;
% Total number of grains in the model
num_grains = 34;

% Define distance between the two twin cutting planes
distance = 4.75;
cut_pln_nrm = [0.5114,-0.4291,-0.7446];
cut_pln(1,:) = [61.3,28,55.1];
cut_pln(2,:) = cut_pln(1,:) + distance*cut_pln_nrm/norm(cut_pln_nrm,2);

neighbor = cell(num_grains,1);
% Read the file containing neighboring grains
fid = fopen(strcat(init_folder,'Neighbors_34.txt'));
for i = 1:num_grains
    tline = fgetl(fid);
    space = find(tline == ' ');
    index = 1;
    for j = 1:length(space)
        grain = str2double(tline(index:space(j)-1));
        index = space(j)+1;
        neighbor{i}(1,j) = grain;
    end
end
fclose(fid);

% We need to make some small changes to var neighbor due to the file/data format
index = length(neighbor{grainID});
for i = 1:grainID-1
    if(isempty(find(neighbor{i}(:) == grainID,1)) == 0)
        index = index + 1;
        neighbor{grainID}(1,index) = i;
    end
end
end
end

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We write the neighboring grain of the selected grain
fprintf(1,strcat('Grain_\',num2str(grainID),' has following neighbors:\n'));
disp(neighbor{grainID})
fprintf(1,strcat('Total of: ',num2str(size(neighbor{grainID},2)),' grains\n'));
disp(' ');

We read the STL file with elements that build Twin Grain Ring ("twin skin")
[vtwin,ftwin] = stlread(strcat(init_folder,'STLs\Grain_1_RING_NEW.stl'));
[vtwin,ftwin] = patchslim(vtwin,ftwin); % Get rid of the duplicated nodes

Now we consider only grains that are neighbors to selected grain (grainID)
[vs,fs] = stlread(strcat(init_folder,'data\Grain_\',num2str(grainID),'.stl'));
for zzz = 1:length(neighbor{grainID})
    % We read surface triangular meshes (STL files) of each grain in order to select those elements that
    % belong to both grains and that are also on the cutting/intersection plane
    [v,f] = stlread(strcat(init_folder,'data\Grain_\',num2str(neighbor{grainID}(1,zzz)),'.stl'));
    [v,f] = patchslim(v,f); %Get rid of the duplicated nodes
    for d = 1:2 % Consider each cutting plane
        % IMPORTANT: You should read deformed STL files
        cut_pln_org = cut_pln(d,:);
        % Normalized plane normal vector
        cut_pln_nrm = cut_pln_nrm/norm(cut_pln_nrm,2);
        pln = zeros(3,3);
        pln(1,:) = cut_pln_org;
        free_term = -dot3(cut_pln_nrm,cut_pln_org);
        qq = find(cut_pln_nrm == 0);
        if(size(qq,2) == 0)
            % We choose x and y and compute z coordinate of the point on the plane
            new_point = [1, 2, -(free_term + cut_pln_nrm(1,1)*1 + cut_pln_nrm(1,2)*2)/cut_pln_nrm(1,3)];
            pln(2,:) = new_point;
            new_point = [1, 5, -(free_term + cut_pln_nrm(1,1)*1 + cut_pln_nrm(1,2)*5)/cut_pln_nrm(1,3)];
            pln(3,:) = new_point;
        elseif(size(qq,2) == 1)
            % We choose x and y and compute z coordinate of the point on the plane
            new_point = [1, 2, -(free_term + cut_pln_nrm(1,1)*1 + cut_pln_nrm(1,2)*2)/cut_pln_nrm(1,3)];
            pln(2,:) = new_point;
            new_point = [1, 5, -(free_term + cut_pln_nrm(1,1)*1 + cut_pln_nrm(1,2)*5)/cut_pln_nrm(1,3)];
            pln(3,:) = new_point;
            elseif(qq == 3)
                % We choose x and z and compute y coordinate of the point on the plane
                new_point = [1, -(free_term + cut_pln_nrm(1,1)*1 + cut_pln_nrm(1,3)*2)/cut_pln_nrm(1,2),2];
                pln(2,:) = new_point;
                new_point = [1, -(free_term + cut_pln_nrm(1,1)*1 + cut_pln_nrm(1,3)*5)/cut_pln_nrm(1,2),5];
                pln(3,:) = new_point;
        end
        elseif(size(qq,2) == 2)
            % We choose y and z and compute x coordinate of the point on the plane
            if(qq == 1) % y,z
                pln(2,:) = [cut_pln_org(1,1) 10 20];
                pln(3,:) = [cut_pln_org(1,1) 50 30];
            elseif(qq == 2)
                pln(2,:) = [10 cut_pln_org(1,2) 20];
                pln(3,:) = [50 cut_pln_org(1,2) 20];
            elseif(qq == 3)
                pln(2,:) = [10 20 cut_pln_org(1,3)];
                pln(3,:) = [50 20 cut_pln_org(1,3)];
        end
elseif(size(qq,2) == 3)
    disp('Plane vector normal is not correctly defined!!')
end

% Number of faces and vertices in the STL file
numfaces = size(f,1);
numverts = size(v,1);

% Calculate face centers and face edge lengths
fc = zeros(numfaces,3);
fe = zeros(numfaces,3);
for i = 1:numfaces
    v1 = v(f(i,1),:); v2 = v(f(i,2),:); v3 = v(f(i,3),:);
    e1 = norm(v2-v1); e2 = norm(v3-v2); e3 = norm(v1-v3);
    fc(i,:) = mean([v1;v2;v3],1);
    fe(i,:) = [e1,e2,e3];
end

% Find the max edge length in the mesh
maxe = max(max(fe));

% Find all faces that are potentially cut by the plane (on distance maxe)
index = 1;
if((d == 2) || (zzz > 1))
    clear tmp1;
end
for i = 1:size(fc,1)
    [~,dist] = determine_side(fc(i,:),cut_pln_nrm,cut_pln_org);
    if(dist < maxe)
        tmp1(index,1) = i;
        index = index + 1;
    end
end

% Initialize e & p left and right
if(d == 1)
    e_left = []; p_left = [];
    cut_left = 1; % by default
elseif(d == 2)
    e_right = []; p_right = [];
    cut_right = 1; % by default
end

if(index == 1)
    continue; % This means that this plane doesn't cut this neighboring grain, so we just proceed further
end
index = 1; tmp = [];
for c = 1:size(tmp1,1)
    if(find(ismember(vs,v(f(tmp1(c,1),1),:),'rows') == 1,1))
        if(find(ismember(vs,v(f(tmp1(c,1),2),:),'rows') == 1,1))
            if(find(ismember(vs,v(f(tmp1(c,1),3),:),'rows') == 1,1))
                % All three nodes are on the grain boundary surface
                tmp(index,1) = tmp1(c,1);
                index = index + 1;
            end
        end
    end
end
end
% If the grain is cut by the plane then cut it, if not, continue with the next grain
if ~isempty(tmp)
    % Remove all faces that are not cut
    fp = f(tmp, :); fc = fc(tmp, :); % f -> fp, fc maybe unnecessary

    ind = [1, 2; 2, 3; 3, 1];
    numfaces = size(fp, 1);
    p = zeros(numfaces * 2, 3);
    e = zeros(numfaces, 3); % Third column is for element (face) ID that was cut
    l = -1;

    for i = 1:numfaces
        % Current face vertex coordinates (3x3 matrix of vertices)
        tri = round([v(fp(i, 1), :); v(fp(i, 2), :); v(fp(i, 3), :)] * 1e10) / 1e10;

        % Check how many vertices are "to the right" of the plane. If 1 or 2 then the face is cut by the plane
        sz1 = 0; sz2 = 0; mind2 = 0;
        for z = 1:3
            [out, dist] = determine_side(tri(z,:), cut_pln_nrm, cut_pln_org);
            if (out == 2)
                sz1 = sz1 + 1;
            end
            if (dist == 0)
                sz2 = sz2 + 1;
                mind2 = z;
            end
        end

        % If the face is cut by the plane, continue, if not jump to the next face
        if (sz1 == 1 || sz1 == 2)
            % Find where (in local line coordinates) the plane intersects the edges of the triangle
            pen = triplapenchkwov(p, tri);
            penind = find(pen > 1e-16 & pen < 1 - 1e-16);

            % Determine the points of the line segments (formed by triangle/cutting plane intersections)
            % These segments should form closed loops, which can be meshed
            switch sz2 % Several cases; If the 0, 1 or 2 vertices lie on the cutting plane, do different things
                case 0
                    % If no vertices lie on the cutting plane, calculate the triangle/plane intersection points
                    v11 = tri(ind(penind(1, 1), :)); v12 = tri(ind(penind(1, 2), :));
                    v21 = tri(ind(penind(2, 1), :)); v22 = tri(ind(penind(2, 2), :));

                    % Determine the vertex coordinates of the intersection points
                    t1 = pen(penind(1)); t2 = pen(penind(2));
                    p1 = v11 + t1 * (v12 - v11); p2 = v21 + t2 * (v22 - v21);
                case 1
                    % If one vertex lies on the plane and cutting plane intersects the triangle, one point of the line
                    % segment is going to have the same coordinate as the vertex on the plane. The second point
                    % coordinate is calculated as triangle/plane intersection.
                    if ~isempty(penind)
                        p1 = tri(mind2(1), :);
                        v11 = tri(ind(penind(1, 1), :)); v12 = tri(ind(penind(1, 2), :));
                        t1 = pen(penind(1));
                        p2 = v11 + t1 * (v12 - v11);
                    end
                case 2
                    % If two vertices lie on the plane, both are written down as line segment points
                    p1 = tri(mind2(1), :);
                    p2 = tri(mind2(2), :);
            end
end
end
\begin{verbatim}

l = l + 2; % counter

% Save the points into a matrix
p(l,:) = p1; p(l+1,:) = p2;

% The connectivity table
e(ceil(l/2),:) = [l,l+1,tmp(i)];
elseif ((sz1 == 0) && (sz2 == 3))
  % In this case, no points are saved, skip to the next grain
  warning(strcat('Problem. There are triangles lying on the cutting plane. Cannot produce a section. Grain number: '),num2str(g));
end
end

% We need to sweep, renumber and connect these element in neighboring grain
index = find(ismember(p, [0 0 0], 'rows') == 1, 1);
p = p(1:index-1,:);
index = find(e(:,1) == 0, 1);
e = e(1:index-1,:);
if ((size(p,1) == 0) || (size(e,1) == 0))
  if (d == 1)
    cut_left = 0;
  else
    cut_right = 0;
  end
  continue; % There is no intersection between this cutting plane and this grain
end

% Remove duplicated nodes.
[p, ~, indexn] = unique(p, 'rows');

maxx = max(max(e(:,1:2))); ee = zeros(size(e,1),3);
for z = 1:maxx
  [row,col] = find(e(:,1:2) == z);
  ee(row,col) = indexn(z); ee(row,3) = e(row,3);
end

% Find additional duplicated nodes (points) that are really close, but because of small numerical % (round-off) error, they are different nodes; NOTE: p is sorted
for z = 1:size(p,1)-1
  if(abs(p(z,1)-p(z+1,1))<1e-6 && abs(p(z,2)-p(z+1,2))<1e-6 && abs(p(z,3)-p(z+1,3))<1e-6)
    p(z,:) = p(z+1,:);
  end
end

[p, indexm, indexn] = unique(p, 'rows'); % Remove duplicated points

e = zeros(size(ee,1),3);
for z = 1:max(max(ee(:,1:2)))
  [row,col] = find(ee(:,1:2) == z);
  for j = 1:length(row)
    e(row(j),col(j)) = indexn(z); e(row(j),3) = ee(row(j),3);
  end
end

% Save elements that are cut by the left cutting plane; intersected nodes as well
if (d == 1) % left side
  e_left = e;
  p_left = p;
end
\end{verbatim}
elseif(d == 2) % right side
  e_right = e;
  p_right = p;
end
end % End of sides (left & right); cutting planes

% Before everything we need to check if we have any intersection
if((size(e_left,1) == 0) && (size(e_right,1) == 0))
  fprintf(1,strcat('First plane is not cutting Grain_',num2str(neighbor{grainID}(1,zzz)),'
'));
  fprintf(1,strcat('Second plane is not cutting Grain_',num2str(neighbor{grainID}(1,zzz)),'
'));
  cut_left = 0;
  cut_right = 0;
end
if((cut_left == 0) && (cut_right == 0)) % There is no intersection with this grain
  fprintf(1,strcat('Grain_',num2str(neighbor{grainID}(1,zzz)),' is done.
'));
  continue; % There is no intersection between this cutting planes and this
end
if((size(e_left,1) == 0)
  fprintf(1,strcat('First plane is not cutting Grain_',num2str(neighbor{grainID}(1,zzz)),'
'));
  cut_left = 0;
end
if((size(e_right,1) == 0)
  fprintf(1,strcat('Second plane is not cutting Grain_',num2str(neighbor{grainID}(1,zzz)),'
'));
  cut_right = 0;
end
%++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
% Now we need to delete these intersected elements and to replace them with the ones from the
% twin ring (belonging to the current grain)
cut_elm = []; % We need to reset cut elements
if(cut_left == 1)
  cut_elm = e_left(:,3);
  % Append vertices first (intersection nodes between the cutting plane and the grain mesh)
  e_left(:,1:2) = e_left(:,1:2) + size(v,1);
  % Update nodeIDs of the intersected nodes - left
  v = [v;p_left];
end
if(cut_right == 1)
  cut_elm = [cut_elm;e_right(:,3)];
  % Append vertices first (intersection nodes between the cutting plane and the grain mesh)
  e_right(:,1:2) = e_right(:,1:2) + size(v,1);
  % Update nodeIDs of the intersected nodes - right
  v = [v;p_right];
end
cut_elm = unique(cut_elm);

% Delete the elements from an element list, but first we memorize them and their nodes to
% reconstruct them later.
f = f(setdiff(1:size(f,1),cut_elm'),:);

% Now we need to find elements from a twin ring that belong to this grain
vtwin_tmp = round(vtwin*10)/10; % Round node coordinates in 2 decimals; temporary variable
v_tmp = round(v*10)/10; % Round node coordinates in 2 decimals; temporary variable

% Find all nodes that they share: Neighboring grain and the twin grain ring
index = 1; tmp = [];
for i = 1:size(ftwin,1) % Loop over all twin ring elements
  if(find(ismember(v_tmp,vtwin_tmp(ftwin(i,1),:),'rows') == 1,1))
    if(find(ismember(v_tmp,vtwin_tmp(ftwin(i,2),:),'rows') == 1,1))
      if(find(ismember(v_tmp,vtwin_tmp(ftwin(i,3),:),'rows') == 1,1))

397
% All three nodes can be found on the grains surface
  tmp(index,1) = i; % Elements that have to be added
  index = index + 1;
end
end
end
delmnt = size(f,1);
for i = 1:size(tmp,1)
  % We need to find appropriate nodeIDs in the grain's nodeID list for each element
  ff1 = find(ismember(v_tmp,vtwin_tmp(ftwin(tmp(i,1),1),:),'rows') == 1,1);
  ff2 = find(ismember(v_tmp,vtwin_tmp(ftwin(tmp(i,1),2),:),'rows') == 1,1);
  ff3 = find(ismember(v_tmp,vtwin_tmp(ftwin(tmp(i,1),3),:),'rows') == 1,1);
  % Add the element into the grain's element list
  f(elmnt,:) = [ff1 ff2 ff3];
delmnt = elmnt + 1;
end

% Overwrite STL file of the neighboring grain
  stlwrite(strcat(init_folder,'data\Grain_\',num2str(neighbor{grainID}(1,zzz)),'.stl'),f,v,'mode','binary');
  fprintf(1,strcat('Grain_\',num2str(neighbor{grainID}(1,zzz)),' is done.\n'));
end % End of neighboring grains

% Matlab script: Python_sweep.m
% This script creates python script that performs node sweep in Abaqus
% First we read STL grain files and generate corresponding INP files for Abaqus import. Lastly we
% perform node merging with prescribed tolerance.

clear all;clc;
init_folder = 'C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6\%deformation2_DD\';
init_inp_folder = 'C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6\%deformation2_DD\INP\';
init_file_name = 'Grain_\';
stl_ext = '.stl';
inp_ext = '.inp';

numstls = 35;
tolerance = 0.001; % a little bit bigger tolerance
% Create folder where all these input files will be saved/stored
mkdir(init_folder,'INP');

% Create *.inp files from *.stl files (ASCII) for each grain
%-------------------------------------------------------------
fprintf(1,'Writing Abaqus grain input files...\n');
for i = 1:numstls
  fprintf(1,'Grain: %d / %d\n',i,numstls);
  stlname = strcat(init_file_name,num2str(i));
  stdaddr = strcat(init_folder,'data\',stlname,stl_ext);
  fid1 = fopen(stdaddr);
  if fid1 ~= -1
    A = textscan(fid1,'%s',1,'Whitespace','\b','delimiter','\r\n\t');
    fclose(fid1);
    A = char(A{1});
    [v,f] = stlread(stdaddr);
  end
  stlwrite(strcat(init_folder,'data\',stlname,'.inp'),v,f,'mode','binary');
  fprintf(1,strcat('Grain_\',num2str(i)),' is done.\n'));
end
inpname = strcat(init_file_name,num2str(i));
inp_addr = strcat(init_inp_folder,inpname,inp_ext);

fid2 = fopen(inp_addr,'w');
fprintf(fid2,'*HEADING
');
fprintf(fid2,'**
');
fprintf(fid2,'** PARTS
');
fprintf(fid2,'**
');
fprintf(fid2,'*Part, name=PART-%i
',i);
fprintf(fid2,'*NODE, NSET=ALL-%i
',i);

for j = 1:length(v)
    fprintf(fid2,'%i, %g, %g, %g
',j,v(j,1),v(j,2),v(j,3));
end

fprintf(fid2,'*ELEMENT,TYPE=S3
');
k = 0;
for j = 1:(length(v)/3)
    fprintf(fid2,'%i, %g, %g, %g
',j,k+1,k+2,k+3);
k = 3*j;
end

fprintf(fid2,'*End Part
');
end

close(fid2);
end

% Create python script that will import all the grains, create part object and perform node % merge/sweep with prescribed tolerance.
fprintf(fid,'Writing Python script...
');
python_name = 'Grain_sweep.py';
fid = fopen(strcat(init_folder,python_name),'wt');

fprintf(fid,'# Python script -> Perform grain node sweep
');
fprintf(fid,'from abaqus import *
');
fprintf(fid,'from abaqusConstants import *
');
fprintf(fid,'from part import *
');
fprintf(fid,'from material import *
');
fprintf(fid,'from section import *
');
fprintf(fid,'from assembly import *
');
fprintf(fid,'from step import *
');
fprintf(fid,'from interaction import *
');
fprintf(fid,'from load import *
');
fprintf(fid,'from mesh import *
');
fprintf(fid,'from job import *
');
fprintf(fid,'from sketch import *
');
fprintf(fid,'from visualization import *
');
fprintf(fid,'from connectorBehavior import *
');
import regionToolset
import os

%
% Change working directory  ->  NOTE: In this location we store our clean/swept grain input files
fprintf(fid,os.chdir("%s")\n',init_folder(1:end-1));
% Create grain model object
GRMModel = mdb.Model(name='"Grain_Model_%u"')\n';
instance=";
for i = 1:numstls
  fprintf(fid,\n    inp_addr = strcat(init_inp_folder,inpname,inp_ext);
    part%u = mdb.models["PART-%u"]\n    nset%u = part%u.sets["ALL-%u"]\n    part%u.mergeNodes(nodes=nset%u, tolerance=0.001)\n    part%u.Set(name='"ElementSet-grain_%u"', elements=part%u.elements)\n    instance%u = mdb.models["Grain_Model_%u"].rootAssembly.Instance(name = "PART-%u", part = part%u)\n    % Copy part object of individual grain to grain model (all grains)
    del mdb.models["Grain_Model_%u"].parts["PART-%u"]\n    % Create instance object
    GRMnodeset = GRMPartALL.nodes\n    % Create node object
    for i = 1:numstls
      % Delete Parts of separate grains
      del mdb.models["Grain_Model_%u"].parts["PART-%u"]\n      toName="NodeSet-Grain_%u"\n      % Create instance from PART-ALL
      % Create instance from PART-ALL
      GRMnodeset = GRMPartALL.nodes\n      % Create node object

400
fprintf(fid, 'GRMPartALL.mergeNodes(nodes=GRMnodeset, tolerance=0.001)n');
% Clean mesh from the short edged elements
fprintf(fid, 'GRMPartALL.cleanMesh(mergeTolerance = 18)n');
% Renumber all nodes in the part
fprintf(fid, 'GRMPartALL.renumberNode(nodes=GRMnodeset, startLabel=1, increment=1)n');
% Renumber all nodes in the part
fprintf(fid, 'GRMPartALL.renumberElement(startLabel=1, increment=1)n');

% Show Grain model part
fprintf(fid, 'session.viewports["Viewport: 1"].setValues(displayedObject=GRMPartALL)n');
fclose(fid);

fprintf(1, 'Complete\n');

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Matlab script: createSTL_GrainModel.m
% This script creates STL grain files from grain model surface mesh, which can be further solid
% meshed in Patran.
clear all; clc;

% Define folder with ABQ grain surface meshes/input files
init_folder = 'C:\Milan\PhD\Research\Mg_TWINSIMULATIONS\step6-6%_deformation2_DD\';
num_grains = 35;
mkdir(strcat(init_folder,'STL'));
fprintf(1, 'Reading Abaqus grain model input file...\n');

% Open grain model input file
fid = fopen(strcat(init_folder,'INP\','AZ31Mg35_cleaned_DD.inp'));
tline = fgetl(fid);
while(strcmp(tline,'*Node') == 0)
tline = fgetl(fid);
end

% Read NODE coordinates
A = textscan(fid,'%u %f %f %f','delimiter',',','Whitespace','\n\t','MultipleDelimsAsOne',1);
nodeID = A{1}(:);
v(:,1) = A{2}(:);
v(:,2) = A{3}(:);
v(:,3) = A{4}(:);

% Read ELEMENT connectivities
A = textscan(fid,'%u %u %u %u %u %u %u %u %u %u %u %u %u %u %u %u ','delimiter',',','Whitespace','\n\t','MultipleDelimsAsOne',1);
model_elementID = A{1}(:);
f(:,1) = A{2}(:);
f(:,2) = A{3}(:);
f(:,3) = A{4}(:);

% Read element and node set definitions
elements = cell(num_grains,1);
nodes = cell(num_grains,1);
for i = 1:num_grains
    tline = fgetl(fid); -- Read *Nset
    A = textscan(fid,'%u %u %u %u %u %u %u %u %u %u %u %u %u %u %u %u ','delimiter',',','Whitespace','\n\t','MultipleDelimsAsOne',1);
    % Find and remove empty cells
    emptyCells = cellfun(@isempty,A);
    A(emptyCells) = [];
end
if(size(A,2) == 3)  \% This means that we have structured data
  nodes{i}(1,1:2) = [A{1}(:) A{2}(:)];
else  \% Unstructured data
  for z = 1:size(A,2)
    nodes{i}(1:size(A{z},1),z) = A{z};
  end
end

\% ELEMENTS
tline = fgetl(fid);  \% Read *Elset
A = textscan(fid,'%u %u %u %u %u %u %u %u %u %u %u %u %u %u %u %u %u %u %u',
\% delimiter','\n','\r','\t','MultipleDelimsAsOne',1);
\% Find and remove empty cells
emptyCells = cellfun(@isempty,A);
A(emptyCells) = [];
if(size(A,2) == 3)  \% This means that we have structured data
  elements{i}(1,1:2) = [A{1}(:) A{2}(:)];
else  \% Unstructured data
  for z = 1:size(A,2)
    elements{i}(1:size(A{z},1),z) = A{z};
  end
end
end
fclose(fid);

fprintf(1,'Writing grain STL files...\n');
\% Setup each grain individually and write them in STL files (ASCII format) for further meshing
for i = 1:num_grains
  fprintf(1,'Grain: %d / %d \n',i,num_grains);
  \%ELEMENTS
  if(size(elements{i},2) == 2)
    elementID = [elements{i}(1,1):1:elements{i}(1,2)]';
  else
    elements_temp = unique(elements{i});
    if(isempty(find(elements{i}==0,1)) == 0)  \% we have 0
      elementID = elements_temp(2:end);  \% skip 0
    else
      elementID = elements_temp;
    end
  end
  \% Create nodeID from elementID
  nodeID = unique(f(elementID,:));
  \% Build vertices and faces
  fgrain = f(elementID,:);  \%
  vgrain = v(nodeID,:);
  NODEID = [nodeID [1:1:size(nodeID,1)]];  \%
  \% Renumber nodes in all faces
  for z = 1:size(fgrain,1)
    for k = 1:3
      fgrain(z,k) = NODEID(find(NODEID(:,1)==fgrain(z,k),1),2);
    end
  end
  \% Define name for stl file
  stl_name = strcat(init_folder,'STL\Grain_',num2str(i),'.stl');

402
FV = struct('vertices',vgrain,'faces',fgrain);
stlwrite(stl_name,FV,'mode','binary');
end

fprintf(1,'Complete\n');

Matlab script: gen_sess_files_mesh_stl_patran.m
This script writes a Patran script that performs 3D solid meshing of the grains (surface meshes)
clc; clear;

Define path where are the STL grain files
init_folder = 'C:\Milan\PhD\Research\SHEAR BANDING Study\MATLAB\Exersize\grains10\';

Patran session/script file name
ses_name = 'mesh_stl_patran.ses';

Define path and name of the Patran database where the meshing will be performed
dbname = 'C:\Milan\PhD\Research\SHEAR BANDING Study\MATLAB\mesh.db';

Default name of the STL grain files generated in DREAM.3D
init_fname = 'Grain_';
stl_ext = '.stl';
neu_ext = '.out';

Define number of grains
numstls = 35;

mxelemset = 5e7;

for i = 1:numstls
    zeross = filename_app_zeros(6,i);
    stlname = strcat(init_fname,num2str(i));
    stladdr = strcat(init_folder,stlname,stl_ext);
    fid2=fopen(stladdr);
    A = textscan(fid2,'%s',1,'Whitespace','\b','delimiter',' \n\t');
    fclose(fid2);
    A = char(A{1});

    Write commands for grain meshing in Patran script language; each grain is meshed individually
    neuexportname = strcat(init_folder,init_fname,zeross,num2str(i),neu_ext);
Matlab script: process_patran_output_nodes_elements.m
This Matlab script performs post-processing of the meshed grains and generates final Abaqus input model along with some other useful text files.

clc; clear;

% Define path where are the Patran output files that contain meshed grains;
init_folder = 'C:\Milan\PhD\Research\SHEAR BANDING Study\MATLAB\Exersize\grains10';
% Folder/path where this script is placed
script_folder = 'C:\Milan\PhD\Research\SHEAR BANDING Study\MATLAB';
init_fname = 'Grain_';
neu_ext = '.out';

% A label which will be appended to create Abaqus input file and some additional files
append_name = 'AZ31_2_TWIN55%_DD';

numcells = 10;
tlrnc = 1e-4;

% Number of grains
numouts = 35;
umnodes = zeros(1,numouts);
numelems = zeros(1,numouts);
setvol = zeros(1,numouts);

coortable = cell(1,numouts);
contable = cell(1,numouts);
elemvol = cell(1,numouts);

for i = 1:numouts
    fprintf(1,'%d / %d
',i,numouts);
    zeross = filename_app_zeros(6,i);
    outname = strcat(init_fname,zeross,num2str(i));
    outaddr = strcat(init_folder,outname,neu_ext);
    fid = fopen(outaddr);
    textscan(fid,'%s',2,'delimiter','n');
    A = textscan(fid,'%*d %*d %*d %*d %*u %*u %*[^n]',1,'Whitespace','b','delimiter','n\r\t','MultipleDelimsAsOne',1);
    numnodes(i) = A{1}{:};
numelemsi = A{2}{:};
    textscan(fid,'%s',1,'delimiter','n');
    A = textscan(fid,'%*f %*f %*f %*f,1,'Whitespace','b','delimiter','n\r','MultipleDelimsAsOne',1);
    coortable{i} = zeros(numnodes(i),3);
    contable{i} = zeros(numelemsi,4);
    elemvol{i} = zeros(numelemsi,1);

    for j = 1:numnodes(i)
        textscan(fid,'%s',1,'delimiter','n');
        A = textscan(fid,'%*f %*f %*f,1,'Whitespace','b','delimiter','n\r','MultipleDelimsAsOne',1);
        coortable{i}(j,1:3) = [A{1}{:},A{2}{:},A{3}{:}];
        textscan(fid,'%s',1,'delimiter','n');
    end
m = 1;
for j = 1:numelemsi
A = textscan(fid,'%*u %u %u %*[^\n]',1,'Whitespace',
\b','delimiter',\n\t','MultipleDelimsAsOne',1);
elmttype = A{2}{:};
if (elmttype == 5)
textscan(fid,'%s',1,'delimiter','\n');  % Skip lines
A = textscan(fid,'%u %u %u %u','%Whitespace',
\b','delimiter',\n\t','MultipleDelimsAsOne',1);
contable{i}(m,:) = [A{1}{:},A{2}{:},A{3}{:},A{4}{:}];

% Tetrahedral element volume calculation
node1i = coortable{i}(contable{i}(m,1),:); node2i = coortable{i}(contable{i}(m,2),:);
node3i = coortable{i}(contable{i}(m,3),:); node4i = coortable{i}(contable{i}(m,4),:);
v1i = node1i-node2i; v2i = node1i-node3i; v3i = node1i-node4i;

elemvol{i}(m) = abs(det([v1i;v2i;v3i]))/6;
else
    textscan(fid,'%s',2,'delimiter','\n');  % Skip lines
end
end

contable{i}(contable{i}(:,1)==0,:) = [];
elemvol{i}(elemvol{i}(:,1)==0,:) = [];
setvol(i) = sum(elemvol{i}(:));
numelems(i) = size(contable{i},1);
fclose(fid);

% Delete some Patran files (byproduct of meshing, but not the ones that contain mesh data)
delete(strcat(script_folder,init_fname,num2str(i),'.bdf'));
delete(strcat(script_folder,init_fname,num2str(i),'.bdf.log'));
delete(strcat(script_folder,init_fname,num2str(i),'.bdf.err'));
delete(strcat(script_folder,init_fname,num2str(i),'.bdf.rej'));
end

modvol = sum(setvol);
umallelems = sum(numelems);
umallnodes = sum(numnodes);
alcoors = zeros(numallnodes,3);
allelems = uint32(zeros(numallelems,4));
m = 0; n = 0;
for i=1:numouts
    alcoors(m+1:m+numnodes(i),:) = coortable{i}(:,:);
    allelems(n+1:n+numallelems(i),:) = contable{i}(:,:) + repmat([m,m,m,m],numallelems(i),1);
    m = m + numnodes(i); n = n + numallelems(i);
end

% Delete duplicated nodes on the grain boundaries
[alcoors,allelems] = patchslim(alcoors, allelems);
umallnodes = size(alcoors,1);

allelems = [linspace(1,numallelems,numallelems)',allelems];
alcoors = [linspace(1,numallnodes,numallnodes)',alcoors];

% Open Abaqus input file and some additional files that contain some useful information
fid = fopen(strcat('ABQtemp_',append_name,'_num2str(numouts)','.inp'),'w');
% File with grain volume fractions
fid19 = fopen(strcat('Volume_Fractions_',append_name,'_num2str(numouts)','.txt'),'w');
% File with grain volumes
fid20 = fopen(strcat('Grain_Volume_',append_name,'_',num2str(numouts),'.txt'),'w');

fprintf(fid,'*Heading\n');
fprintf(fid,'*Part, name=part1\n');
fprintf(fid,'*Node\n');
fprintf(fid,'%7u,%13.6f,%13.6f,%13.6f\n',allcoors);
fprintf(fid,'*Element, type=C3D4\n');
fprintf(fid,'%9u,%9u,%9u,%9u,%9u\n',allelems);

n = 0;
offset = 0; % Option to make an offset in Section, Material, ElementSet definitions
for i=1:numouts
    zeross = filename_app_zeros(4,i+offset);
    grainnumstr = strcat(zeross,num2str(i+offset));
    fprintf(fid,'*Elset, elset=grain-%s, generate\n',grainnumstr);
    fprintf(fid,'%9u,%9u,1\n',n+1,n+numelems(i));
    fprintf(fid,'*Solid Section, elset=grain-%s, material=mgrain-%s\n',grainnumstr,grainnumstr);
    fprintf(fid,'**Elset volume fraction: %6f\n',setvol(i)/modvol);
    fprintf(fid19,'%6f\n',setvol(i)/modvol);
    fprintf(fid20,'%6f\n',setvol(i));
    n = n+numelems(i);
end
fprintf(fid,'*End Part\n');

for i=1:numouts
    zeross = filename_app_zeros(4,i+offset);
    grainnumstr = strcat(zeross,num2str(i+offset));
    fprintf(fid,'*Material, name=mgrain-%s\n',grainnumstr);
    fprintf(fid,'*USER MATERIAL, CONSTANTS=1\n');
    fprintf(fid,'%u\n',i+offset);
    fprintf(fid,'*DEPVAR\n');
    fprintf(fid,'650\n'); % Prescribed number of state variables
end
fclose(fid);
fclose(fid19);
fclose(fid20);

% Write a text file that contains number of elements per element set/grain
fid23 = fopen(strcat('NumElemSet_',append_name,'_',num2str(numouts),'.txt'),'w');
for i = 1:length(numelems)
    fprintf(fid23,'%u\n',numelems(1,i));
end
fclose(fid23);

% Write element volume fractions/normalized weights - for texture plotting
X = load(strcat(script_folder,'NumElemSet_',append_name,'_',num2str(numouts),'.txt'));

% Compute element volume fractions
element_fraction = zeros(length(allelems),1);
l = 1;
for k = 1:numouts
    for q = 1:X(k,1)
        element_fraction(l,1) = elemvol{k}(q)/modvol;
        l = l + 1;
    end
end
% Write element volume fractions
fid7 = fopen(strcat('Element_fractions_',append_name,'.txt'),'w');
for i = 1:length(element_fraction)
    fprintf(fid7,'%.9f
',element_fraction(i,1));
end
fclose(fid7);

% Matlab script: mesh2mesh_mapping.m
% This script maps the values between the state variables in the "old" mesh (before incepting a twin) % and the "new" mesh (after introducing the twin grain). The mapping is performed based on the % mutual proximity of their element's centroids and it is performed per grain.
clear all; clc;

% Define initial folder with FE model/mesh
init_folder = 'C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6%_deformation2_DD\INP\';
num_grains1 = 34; % number of grains in the OLD mesh
num_grains2 = 35; % number of grains in the NEW mesh

% Define the name of the OLD FEA input model: MESH1
grain_file1 = 'AZ31Mg34_TWIN40%_DD_5p6%.inp';
% Define name of the NEW FEA input model: MESH2
grain_file2 = 'AZ31_2_TWIN55%_DD_35.inp';

%**************************************************************************
% --- FIRST MESH => MESH1
fid = fopen(strcat(init_folder,grain_file1));
tline = fgetl(fid);
while(strcmp(tline,'*Node')==0)
tline = fgetl(fid);
end

% Read NODE coordinates
A = textscan(fid,'%u %f %f %f','delimiter',',','Whitespace','
\rt','MultipleDelimsAsOne',1);
nodeID = A{1}(:);
v1 = [A{2}(:) A{3}(:) A{4}(:)];

% Read ELEMENT connectivities
tline = fgetl(fid); % skip first line (e.g. *Element, type=C3D4)
A = textscan(fid,'%u %u %u %u %u','delimiter',',','Whitespace','
\rt','MultipleDelimsAsOne',1);
elementID = A{1}(:);
f1 = [A{2}(:) A{3}(:) A{4}(:) A{5}(:)];

% Read ELEMENT SET definitions (GRAINS)
grain_elements1 = cell(1,num_grains1);
for i = 1:num_grains1
tline = fgetl(fid); % skip line (e.g. *Elset, elset=GRAIN-0001, generate)
A = textscan(fid,'%u %u %u %u %u','delimiter',',','Whitespace','
\rt','MultipleDelimsAsOne',1);
grainID = i;
grain_elements1{i} = [A{1}(1):1:A{2}(1)];
end
fclose(fid);

% Compute element centroids in the old mesh
centroids1 = cell(1,num_grains1);
for i = 1:num_grains1
    for j = 1:size(grain_elements1{i},1)
element = grain_elements1{i}(j,1);
xc = (v1(f1(element,1),1) + v1(f1(element,2),1) + v1(f1(element,3),1) + v1(f1(element,4),1))/4;
yc = (v1(f1(element,1),2) + v1(f1(element,2),2) + v1(f1(element,3),2) + v1(f1(element,4),2))/4;
zc = (v1(f1(element,1),3) + v1(f1(element,2),3) + v1(f1(element,3),3) + v1(f1(element,4),3))/4;
centroids1{i}(j,1:3) = [xc yc zc];
end
end

%****************************************************************
% --- SECOND MESH => MESH2
% Read data for the second mesh: MESH2
fid = fopen(strcat(init_folder,grain_file2));
tline = fgetl(fid); while(strcmp(tline,'*Node')==0) tline = fgetl(fid); end
% Read NODE coordinates
A = textscan(fid,'%u %f %f %f','delimiter','\n\t','Whitespace','\n\t','MultipleDelimsAsOne',1);
nodeID = A{1}(:);
v2 = [A{2}(:) A{3}(:) A{4}(:)];

% Read ELEMENT connectivities
tline = fgetl(fid); A = textscan(fid,'%u %u %u %u %u','delimiter','\n\t','Whitespace','\n\t','MultipleDelimsAsOne',1);
elementID = A{1}(:);
f2 = [A{2}(:) A{3}(:) A{4}(:) A{5}(:)];

% Read NODE and ELEMENT SET definitions (GRAINS)
grain_elements2 = cell(1,num_grains2);
node_elements2 = cell(1,num_grains2);
for i = 1:num_grains2
tline = fgetl(fid); A = textscan(fid,'%u %u %u %u %u','delimiter','\n\t','Whitespace','\n\t','MultipleDelimsAsOne',1);
  grainID = i;
  grain_elements2{i} = [A{1}(1):1:A{2}(1)];
end
close(fid);

% Compute element centroids in the new mesh
centroids2 = cell(1,num_grains2);
for i = 1:num_grains2
  for j = 1:size(grain_elements2{i},1)
    element = grain_elements2{i}(j,1);
    xc = (v2(f2(element,1),1) + v2(f2(element,2),1) + v2(f2(element,3),1) + v2(f2(element,4),1))/4;
    yc = (v2(f2(element,1),2) + v2(f2(element,2),2) + v2(f2(element,3),2) + v2(f2(element,4),2))/4;
    zc = (v2(f2(element,1),3) + v2(f2(element,2),3) + v2(f2(element,3),3) + v2(f2(element,4),3))/4;
    centroids2{i}(j,1:3) = [xc yc zc];
  end
end

% We are performing mapping grain-to-grain. We take all elements from each grain from the new
% mesh and then we determine which element in the old mesh is the most closest to that element.
% NOTE: MESH1 and MESH2 have to fulfill the same volume

grain_elements1{35} = grain_elements1{1};
centroids1{35} = centroids1{1};
fid = fopen(strcat(init_folder,'lista.txt'),'wt');
fid11 = fopen(strcat(init_folder,'lista_grain1.txt'),'wt');
for i = 1:num_grains2
    num_elem = size(grain_elements1{i},1); % Number of elements in the current grain
    for j = 1:size(grain_elements2{i},1)
        distance = centroids1{i}(:,1:3) - repmat(centroids2{i}(j,1:3),[],num_elem);
        dnorm = sqrt(sum(distance.*distance,2));
        index = find(dnorm == min(dnorm),1);
        fprintf(fid,'%u\n',grain_elements1{i}(index,1)); % We write the element ID (from the old mesh) into the list
    end
    fprintf(fid11,'%u\n',grain_elements1{i}(index,1)); % We are writing one more txt file - mapped elementIDs only for selected (parent) grain.
    if(i == 1) % Selected parent grain (in the center of the grain model) has ID=1
        fprintf(fid11,'%u\n',grain_elements1{i}(index,1)); % We will use this file to map activities and Fpi inside the grain.
        end
    end
fprintf(1,'Complete.\n');fclose(fid);fclose(fid11);

#Python script: Extract_texture.py
#This script extracts texture (crystal orientations) from the FEA granular model

1. from odbAccess import *
2. from abaqusConstants import *
3. from odbMaterial import *
4. from odbSection import *
5. odb = openOdb(path='C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6%_deformation_DD\AZ31Mg34_6_TWIN40%_6_DD.odb')
6. step1 = odb.steps.values()[2] # STEP: Apply pressure
7. # Define frame to extract
8. lastFrame = odb.steps[step1.name].frames[7]
9. instance = odb.rootAssembly.instances['PART1-1']
10. phi1 = lastFrame.fieldOutputs['SDV552'].getSubset(region = instance)
11. PHI = lastFrame.fieldOutputs['SDV553'].getSubset(region = instance)
12. phi2 = lastFrame.fieldOutputs['SDV554'].getSubset(region = instance)
13. #/////write texture ///////////
14. fobj = open("C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6%_deformation_DD\ODB_data\TEXTURE_OUT_AZ31_5p6%_DD.txt", 'w')
15. for v in phi1.values:
16.    fobj.write('%3.2f\n' % v.data)
17. for v in PHI.values:
18.    fobj.write('%3.2f\n' % v.data)
19. for v in phi2.values:
20.    fobj.write('%3.2f\n' % v.data)
21. fobj.close()
22. odb.close()
# Python script: Extract_CrssDisl_AZ31.py
# This script extracts values of critical resolved shear stress (CRSS) and dislocation densities (DD) # from the FEA granular model.

```python
# from odbAccess import *
from abaqusConstants import *
from odbMaterial import *
from odbSection import *

# AZ31
odb = openOdb(path='C:\Milan\PhD\Research\Mg_TWINSIMULATIONS\step6-6%_deformation_DD\AZ31Mg34_6_TWINSIMULATIONS\6%_deformation_DD.odb')
step1 = odb.steps.values()[2]  # STEP: Apply pressure

# Define frame to extract
lastFrame = odb.steps[step1.name].frames[7]
instance = odb.rootAssembly.instances['PART1-1']
GrainSet = instance.elementSets['GRAIN-0001']

#/////// export CRSS - SLIP + TWIN /////////
CRSS1 = lastFrame.fieldOutputs['SDV64'].getSubset(region=instance)
CRSS2 = lastFrame.fieldOutputs['SDV65'].getSubset(region=instance)
CRSS3 = lastFrame.fieldOutputs['SDV66'].getSubset(region=instance)
CRSS4 = lastFrame.fieldOutputs['SDV67'].getSubset(region=instance)
CRSS5 = lastFrame.fieldOutputs['SDV68'].getSubset(region=instance)
CRSS6 = lastFrame.fieldOutputs['SDV69'].getSubset(region=instance)
CRSS7 = lastFrame.fieldOutputs['SDV70'].getSubset(region=instance)
CRSS8 = lastFrame.fieldOutputs['SDV71'].getSubset(region=instance)
CRSS9 = lastFrame.fieldOutputs['SDV72'].getSubset(region=instance)
CRSS10 = lastFrame.fieldOutputs['SDV73'].getSubset(region=instance)
CRSS11 = lastFrame.fieldOutputs['SDV74'].getSubset(region=instance)
CRSS12 = lastFrame.fieldOutputs['SDV75'].getSubset(region=instance)

#/////// export CRSTW - TWINS //////////////
CRSTW1 = lastFrame.fieldOutputs['SDV303'].getSubset(region=instance)
CRSTW2 = lastFrame.fieldOutputs['SDV304'].getSubset(region=instance)
CRSTW3 = lastFrame.fieldOutputs['SDV305'].getSubset(region=instance)
CRSTW4 = lastFrame.fieldOutputs['SDV306'].getSubset(region=instance)
CRSTW5 = lastFrame.fieldOutputs['SDV307'].getSubset(region=instance)
CRSTW6 = lastFrame.fieldOutputs['SDV308'].getSubset(region=instance)
CRSTW7 = lastFrame.fieldOutputs['SDV309'].getSubset(region=instance)
CRSTW8 = lastFrame.fieldOutputs['SDV310'].getSubset(region=instance)
CRSTW9 = lastFrame.fieldOutputs['SDV311'].getSubset(region=instance)
CRSTW10 = lastFrame.fieldOutputs['SDV312'].getSubset(region=instance)
CRSTW11 = lastFrame.fieldOutputs['SDV313'].getSubset(region=instance)
CRSTW12 = lastFrame.fieldOutputs['SDV314'].getSubset(region=instance)

fobj = open('C:\Milan\PhD\Research\Mg_TWINSIMULATIONS\step6-6%_deformation_DD\ODB_data\CRSS_AZ31_OUT_5p6%_DD.txt', 'w')

for v in CRSS1.values:
    fobj.write('%5.5f
' % v.data)
for v in CRSS2.values:
    fobj.write('%5.5f
' % v.data)
for v in CRSS3.values:
    fobj.write('%5.5f
' % v.data)
```

55. for v in CRSS4.values:
56.     fobj.write('%5.5f
' % v.data)
57. for v in CRSS5.values:
58.     fobj.write('%5.5f
' % v.data)
59. for v in CRSS6.values:
60.     fobj.write('%5.5f
' % v.data)
61. for v in CRSS7.values:
62.     fobj.write('%5.5f
' % v.data)
63. for v in CRSS8.values:
64.     fobj.write('%5.5f
' % v.data)
65. for v in CRSS9.values:
66.     fobj.write('%5.5f
' % v.data)
67. for v in CRSS10.values:
68.     fobj.write('%5.5f
' % v.data)
69. for v in CRSS11.values:
70.     fobj.write('%5.5f
' % v.data)
71. for v in CRSS12.values:
72.     fobj.write('%5.5f
' % v.data)
73.
74. # Twinning
75. for v in CRSSTW1.values:
76.     fobj.write('%5.5f
' % v.data)
77. for v in CRSSTW2.values:
78.     fobj.write('%5.5f
' % v.data)
79. for v in CRSSTW3.values:
80.     fobj.write('%5.5f
' % v.data)
81. for v in CRSSTW4.values:
82.     fobj.write('%5.5f
' % v.data)
83. for v in CRSSTW5.values:
84.     fobj.write('%5.5f
' % v.data)
85. for v in CRSSTW6.values:
86.     fobj.write('%5.5f
' % v.data)
87. for v in CRSSTW7.values:
88.     fobj.write('%5.5f
' % v.data)
89. for v in CRSSTW8.values:
90.     fobj.write('%5.5f
' % v.data)
91. for v in CRSSTW9.values:
92.     fobj.write('%5.5f
' % v.data)
93. for v in CRSSTW10.values:
94.     fobj.write('%5.5f
' % v.data)
95. for v in CRSSTW11.values:
96.     fobj.write('%5.5f
' % v.data)
97. for v in CRSSTW12.values:
98.     fobj.write('%5.5f
' % v.data)
99. fobj.close()
100.
101.
102. # //////////////////////////////////////////////////////////////////////////
103. DISLOCATION DENSITIES
104. RHO_S1 = lastFrame.fieldOutputs['SDV256'].getSubset(region = instance)
105. RHO_S2 = lastFrame.fieldOutputs['SDV257'].getSubset(region = instance)
106. RHO_S3 = lastFrame.fieldOutputs['SDV258'].getSubset(region = instance)
107. RHO_DEB = lastFrame.fieldOutputs['SDV259'].getSubset(region = instance)
108.
109. # Substructure/Debris dislocations
110. fobj = open("C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6\ deformation_DD\ ODB_data\ RHO_DEB_AZ31_OUT_Sp6_ DD.txt", 'w')
111. for v in RHO_DEB.values:
112.     fobj.write('%f
' % v.data)
113. fobj.close()
114.
115. # Forest dislocations - 3 slip modes
from odbAccess import *
from abaqusConstants import *
from odbMaterial import *
from odbSection import *

# AZ31
odb = openOdb(path='C:\Milan\PhD\Research\Mg_TWINSIMULATIONS\step6-6%_deformation_DD\AZ31Mg34_6_TWIN40%_6%_DD.odb')
step1 = odb.steps.values()[2]  # STEP: Apply pressure

# Define frame to extract
lastFrame = odb.steps[step1.name].frames[7]
instance = odb.rootAssembly.instances['PART1-1']
GrainSet = instance.elementSets['GRAIN-0001']

# /////////// export ACTIVITIES - SLIP + TWIN /////////// ACCUMULATED VALUES
# SLIP activities
ACT_SL1 = lastFrame.fieldOutputs['SDV581'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')
ACT_SL2 = lastFrame.fieldOutputs['SDV582'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')
ACT_SL3 = lastFrame.fieldOutputs['SDV583'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')
ACT_SL4 = lastFrame.fieldOutputs['SDV584'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')
ACT_SL5 = lastFrame.fieldOutputs['SDV585'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')
ACT_SL6 = lastFrame.fieldOutputs['SDV586'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')
ACT_SL7 = lastFrame.fieldOutputs['SDV587'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')
ACT_SL8 = lastFrame.fieldOutputs['SDV588'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')
ACT_SL9 = lastFrame.fieldOutputs['SDV589'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')
ACT_SL10 = lastFrame.fieldOutputs['SDV590'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')
ACT_SL11 = lastFrame.fieldOutputs['SDV591'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')
ACT_SL12 = lastFrame.fieldOutputs['SDV592'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')
# TWIN activities

ACT_TW1 = lastFrame.fieldOutputs['SDV593'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')

ACT_TW2 = lastFrame.fieldOutputs['SDV594'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')

ACT_TW3 = lastFrame.fieldOutputs['SDV595'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')

ACT_TW4 = lastFrame.fieldOutputs['SDV596'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')

ACT_TW5 = lastFrame.fieldOutputs['SDV597'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')

ACT_TW6 = lastFrame.fieldOutputs['SDV598'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')

ACT_TW7 = lastFrame.fieldOutputs['SDV599'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')

ACT_TW8 = lastFrame.fieldOutputs['SDV600'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')

ACT_TW9 = lastFrame.fieldOutputs['SDV601'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')

ACT_TW10 = lastFrame.fieldOutputs['SDV602'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')

ACT_TW11 = lastFrame.fieldOutputs['SDV603'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')

ACT_TW12 = lastFrame.fieldOutputs['SDV604'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4')

fobj = open("C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6%_deformation_DD\ODB_data\ACTIVITIES_AZ31_OUT_5p6%_DD.txt", 'w')

# Slip

for v in ACT_SL1.values:
    fobj.write('%2.8fn' % v.data)

for v in ACT_SL2.values:
    fobj.write('%2.8fn' % v.data)

for v in ACT_SL3.values:
    fobj.write('%2.8fn' % v.data)

for v in ACT_SL4.values:
    fobj.write('%2.8fn' % v.data)

for v in ACT_SL5.values:
    fobj.write('%2.8fn' % v.data)

for v in ACT_SL6.values:
    fobj.write('%2.8fn' % v.data)

for v in ACT_SL7.values:
    fobj.write('%2.8fn' % v.data)

for v in ACT_SL8.values:
    fobj.write('%2.8fn' % v.data)

for v in ACT_SL9.values:
    fobj.write('%2.8fn' % v.data)

for v in ACT_SL10.values:
    fobj.write('%2.8fn' % v.data)

for v in ACT_SL11.values:
    fobj.write('%2.8fn' % v.data)

for v in ACT_SL12.values:
    fobj.write('%2.8fn' % v.data)

# Twin

for v in ACT_TW1.values:
    fobj.write('%2.8fn' % v.data)

for v in ACT_TW2.values:
    fobj.write('%2.8fn' % v.data)

for v in ACT_TW3.values:
```python
fobj.write('%2.8f
' % v.data)
for v in ACT_TW4.values:
fobj.write('%2.8f
' % v.data)
for v in ACT_TW5.values:
fobj.write('%2.8f
' % v.data)
for v in ACT_TW6.values:
fobj.write('%2.8f
' % v.data)
for v in ACT_TW7.values:
fobj.write('%2.8f
' % v.data)
for v in ACT_TW8.values:
fobj.write('%2.8f
' % v.data)
for v in ACT_TW9.values:
fobj.write('%2.8f
' % v.data)
for v in ACT_TW10.values:
fobj.write('%2.8f
' % v.data)
for v in ACT_TW11.values:
fobj.write('%2.8f
' % v.data)
for v in ACT_TW12.values:
fobj.write('%2.8f
' % v.data)
fobj.close()
odb.close()

#==============================================================
# Python script: Extract_Fpi.py
# This script extracts values of accumulated shear strains for each particular slip and twin crystallographic system in the FEA granular model.

from odbAccess import *
from abaqusConstants import *
from odbMaterial import *
from odbSection import *

# AZ31
odb = openOdb(path='C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6\deformation_DD\AZ31Mg34_6_TWIN40%_6\DD.odb')
step1 = odb.steps.values()[2]  # STEP: Apply pressure

# Define frame to extract
lastFrame = odb.steps[step1.name].frames[7]
instance = odb.rootAssembly.instances['PART1-1']
GrainSet = instance.elementSets['GRAIN-0001']
GrainNumElem = len(GrainSet.elements)

# export ACTIVITIES - SLIP + TWIN

# SLIP activities
FPI_1 = lastFrame.fieldOutputs['SDV55'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4').values
FPI_2 = lastFrame.fieldOutputs['SDV56'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4').values
FPI_3 = lastFrame.fieldOutputs['SDV57'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4').values
FPI_4 = lastFrame.fieldOutputs['SDV58'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4').values
FPI_5 = lastFrame.fieldOutputs['SDV59'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4').values
```

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25. `FPI_6 = lastFrame.fieldOutputs['SDV60'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4').values`
26. `FPI_7 = lastFrame.fieldOutputs['SDV61'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4').values`
27. `FPI_8 = lastFrame.fieldOutputs['SDV62'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4').values`
28. `FPI_9 = lastFrame.fieldOutputs['SDV63'].getSubset(region=GrainSet, position=INTEGRATION_POINT, elementType='C3D4').values`
29. 
30. # This is performed only for this one grain - element set
31. `fobj = open("C:\Milan\PhD\Research\Mg_TWIN\SIMULATIONS\step6-6_deformation_DD\ODB_data\Fpi_AZ31_OUT_5p6%_DD.txt", 'w')`
32. 
33. # Write Fp for each element in the twinned grain. Values are placed by columns.
34. `for v in range(0, GrainNumElem):
   fobj.write('%.5f\n' % FPI_1[v].data)
   fobj.write('%.5f\n' % FPI_2[v].data)
   fobj.write('%.5f\n' % FPI_3[v].data)
   fobj.write('%.5f\n' % FPI_4[v].data)
   fobj.write('%.5f\n' % FPI_5[v].data)
   fobj.write('%.5f\n' % FPI_6[v].data)
   fobj.write('%.5f\n' % FPI_7[v].data)
   fobj.write('%.5f\n' % FPI_8[v].data)
   fobj.write('%.5f\n' % FPI_9[v].data)
   fobj.close()
35. odb.close()`