STRAIN PATH SENSITIVE POLYCRYSTAL PLASTICITY CONSTITUTIVE MODELS WITHIN FINITE ELEMENTS FOR METAL FORMING SIMULATIONS

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STRAIN PATH SENSITIVE POLYCRYSTAL PLASTICITY CONSTITUTIVE MODELS WITHIN FINITE ELEMENTS FOR METAL FORMING SIMULATIONS

BY

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DISSERTATION

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

Doctor of Philosophy
in
Mechanical Engineering

December, 2018
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On September 14th, 2018

Original approval signatures are on file with the University of New Hampshire Graduate School.
DEDICATION

This thesis is dedicated to my family and friends.
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ABSTRACT

STRAIN PATH SENSITIVE POLYCRYSTAL PLASTICITY CONSTITUTIVE MODELS WITHIN FINITE ELEMENTS FOR METAL FORMING SIMULATIONS

by

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University of New Hampshire, September, 2018

An optimal sheet metal forming process shapes a metal part to the accurate geometry, while avoiding instabilities causing localization of deformation and fracture. Understanding the underlying mechanisms responsible for deformation localization and deviation of final part geometry from the desired geometry facilitates the search for the optimal sheet metal forming process. Accurate modeling of forming processes allows prediction of the formed part shape and can provide insight into the material behavior by interpretation of experimental measurements and prediction of variables not accessible to experimental characterization. In this work, a micromechanical material model is coupled with finite elements to create a multi-scale model of a metal forming process. In addition, extensions to the micromechanical material model have been implemented to accurately describe the material behavior during complex deformation paths observed during forming processes. An implicit numerical integration procedure of the micromechanical model equations is developed for purpose of reducing high computational times characteristic for multi-scale simulations. The developed material model is calibrated against experimental data and used in a finite element simulation of
a cup drawing forming process of aluminum alloy AA6022-T4 to predict the formed cup geometry. Furthermore, the multi-scale modeling approach is utilized to study the mechanics of bending under tension deformation state as a mechanism for postponing the instabilities in deformation processes. The model of the process is capable of capturing the experimentally observed trends in mechanical response and offers insight into the microstructure evolution. The developed modeling framework is computationally intensive, but feasible.
CHAPTER 1:
Overview

1. Introduction

In metal forming, metal parts are mechanically deformed to their final shape. Sheet metal forming is widely used in automotive industry to form parts without loss of material. The desired final part shape dictates the tool geometry and the blank geometry. The relationship between the final part shape, the tool geometry and the blank geometry is often times obscure and highly dependent on the material behavior, in particular the material anisotropy and strain path sensitivity. Due to presence of a preferred crystal orientation, materials can exhibit anisotropy in mechanical response, both in elastic and plastic regimes. The anisotropy evolves with the plastic deformation and is driven by the texture and the microstructure evolution. A change of straining direction causes a change in the material mechanical response, often including transient behaviors characteristic to the strain path change applied. The behavior is referred to as the strain path sensitivity and is governed by the evolution of the microstructure. In addition, the elastic deformation of the sheet metal part, after removing from tools, referred to as the springback, can have a significant effect on the final part shape [1].

Accurate prediction of the final part geometry allows efficient optimization of the forming process. Since the final part shape is a function of the initial material state, the blank geometry and the tool geometry, optimization of any of these variables is possible. For instance, for a given tool geometry and material of the part, the blank
geometry can be optimized to give the minimum deviation between the desired and true final part geometry. Such optimization reduces waste of material and resources in subsequent forming processes. Therefore, accurate models of the sheet metal forming processes with predictive capabilities are highly desirable in order to perform the optimization in an efficient manner.

During the forming process, parts can undergo large plastic deformation. Therefore, one of the basic requirements for material to be used in the sheet metal forming process is sufficient ductility. Unfortunately, light materials with high strength, such as aluminum alloy AA6022-T4, are not as ductile as e.g. low carbon steel, and therefore their application in the automotive industry is limited. In this case, rather than changing the initial material state or the blank geometry, the deformation process can be modified to prolong the plastic deformation and prevent fracture. A class of forming processes, termed incremental sheet forming (ISF) processes, relies on forming of small volume of a part at a given time instant to postpone the strain localization and fracture, thereby increasing the formability [2]. Bending under tension has been identified as one of the mechanisms for increasing the formability [2]. The mechanism has been studied by means of an ordinary tension test performed on a specimen simultaneously subjected to three point bend by rollers moving along the gage length of the specimen. Such a test is referred to as the continuous bending under tension (CBT) test [3]. The CBT experimental setup suppresses strain localization (necking) and allows elongation of the specimen to exceed that obtained during a conventional tension test. The CBT test was studied experimentally [4-6] and theoretically [2, 7], with the aim of understanding the material behavior and mechanics of the process. Modeling of the
CBT process has been directed towards understanding of the mechanics at the macroscopic level, where the spatial resolution is at the order of $10^{-1}$ mm [5, 8, 9]. Model predictions of the microstructure evolution and the crystal level behavior i.e. predictions at a lower length scale, are lacking in the literature. Such predictions can facilitate better understanding of the CBT processes.

Although seemingly different, the tasks of achieving accurate final part geometry and understanding material behavior during the CBT test can benefit from sophisticated micromechanical material models coupled with standard finite element software. Such material models, calibrated on standard mechanical tests, can provide accurate predictions of the deformed part shape [10, 11] and offer some insight into the texture and microstructure evolution during the deformation processes [12]. The major drawback of micromechanical material models is their complexity, resulting in a high computational cost compared to phenomenological material models.

The aim of this work is development of a strain path sensitive micromechanical material model coupled with finite elements for efficient and accurate simulation of metal forming processes. The model is applied to predict the formed part geometry and to simulate the CBT test. For the aim and scope of the work, the following objectives are identified:

- Polycrystal plasticity within finite elements: mathematical formulation, numerical integration and coupling with finite elements (Chapters 2 and 3)
- Strain path sensitive hardening law for polycrystal plasticity (Chapters 4 and 5)
- Case study 1: cup drawing of aluminum alloy AA6022-T4 (included in Chapter 2)
Case study 2: polycrystal plasticity simulation of the CBT test on aluminum alloy AA6022-T4 (Chapter 6)

The thesis is organized in the following way. Rest of the Chapter 1 is dedicated to description of main results and conclusions from the thesis. Identified objectives and minor and major results are described in detail in Chapters 2 through 6. Chapter 2 is a preprint of a journal article submitted for publication, while Chapters 3 through 5 are reprints of published journal articles. Chapter 6 has not been submitted for publication. Finally, main results from this thesis are summarized and directions for further research are provided Chapter 7.

2. Polycrystal plasticity within finite elements: mathematical formulation, numerical integration and coupling with finite elements

In order to define the spatial distribution of displacement in the part under applied loads and displacements, the equilibrium, compatibility and constitutive relations need to be satisfied throughout the volume of the part. The applied displacements and forces define the boundary conditions on the surface of the part, which vary during the time of the forming process. The problem is solved with the finite element method. The finite element method uses the discretized form of the equilibrium equations expressed in function of the vector of nodal displacements:

\[ \mathbf{R}(\mathbf{u}) - \mathbf{F}(\mathbf{u}) = \mathbf{M}\ddot{\mathbf{u}}, \]  

where \( \mathbf{R} \) is the vector of external nodal forces, \( \mathbf{F} \) is the vector of internal forces originating from element stresses, \( \mathbf{u} \) is the vector of nodal displacements and \( \mathbf{M} \) is the mass matrix. Inertial effects during the forming process are not relevant and can be
disregarded, resulting in the static equilibrium at any time instant during the deformation process and Eq. (1) reduces to a system of non-linear equations instead of a system of differential equations in nodal displacements. The deformable part during the forming process goes through series of equilibrium states, starting from the initial unstressed state. The equilibrium states are defined for specific time instances determined by the adopted time incrimination procedure. The task of the FE procedure is to find the vector of nodal displacements, \( \mathbf{u} \), satisfying Eq. (1) at each specified time instant, using the variables from the most recent equilibrium state.

The Eq. (1) establishes the equilibrium at the macroscopic length scale. Inclusion of the microstructure evolution and material behavior at lower length scale is introduced through the constitutive relation. The constitutive relations define the stress-strain response of the material, meaning that for the imposed strain history, the stress history can be evaluated and vice versa. The constitutive law in Eq. (1) is contained within the vector of internal forces, \( \mathbf{F} \). In the finite element formulation used here the constitutive relation is the calculation of the increment in stress, \( \Delta \sigma \), in terms of the increment in strain between two equilibrium states, \( \Delta \varepsilon \). In this work the material stress-strain response at macroscopic level is defined using a crystal plasticity micromechanical modeling.

In this section an implicit algorithm is developed to integrate the set of crystal plasticity equations used as constitutive law. The implicit integration algorithm is compared with the explicit integration algorithm developed in [13, 14]. The motivation behind the development of the implicit algorithm is reduction of computational time by using fewer sub-steps in implicit integration procedure. Finally, the coupling of the
integration algorithm with finite elements is discussed. Detailed description and validation of the numerical integration procedure and its coupling with finite elements is presented in Chapter 2. Special considerations arising from coupling of the crystal plasticity constitutive law with the shell elements are discussed in Chapter 3.

2.1 Crystal plasticity micromechanical modeling

Polycrystalline materials are heterogeneous materials consisting of single crystals. The smallest volume of the body having the response representative of the continuum is called a representative volume element (RVE) [15]. The constitutive relation for the polycrystalline material is defined for the RVE.

The constitutive relation for single crystals making the RVE is well defined and for imposed strain history, the stress history can be calculated. The transition from the single crystal constitutive law to the overall constitutive behavior of collection of crystals is performed by averaging procedures [16]. The average value of a quantity \( q \) is calculated as [16]:

\[
Q = \langle q \rangle = \frac{1}{V} \int_V q \, dV
\]  

(2)

where \( Q \) is the averaged quantity \( q \), \( V \) is the volume of the RVE and \( \langle \quad \rangle \) denotes volume average.

In what follows, first, the continuum equations defining the constitutive law of single crystals in rate form are presented, followed by the outline of the RVE constitutive relations in the rate form. All continuum equations are written in the current configuration. Next, the implicit numerical integration of the rate equations is
summarized. The implicit numerical integration is validated with the explicit integration procedure in terms of stress-strain response and texture evolution. Finally, the comparison of computational times between the implicit and explicit integration procedures is summarized.

2.1.1 Elasto-plastic self-consistent modeling framework

2.1.1.1 Single crystal constitutive law

Single crystals occupy certain volume in polycrystalline RVE. During the deformation process every point in this volume will move. The current position of each point is given by (unknown) motion function:

\[ \mathbf{x} = \chi(\mathbf{X}, t) \quad (3) \]

where \( \mathbf{x} \) is a position vector in the current configuration, \( \mathbf{X} \) is a position vector in the reference configuration and \( t \) is the current time. The current velocity of a material point identified with \( \mathbf{X} \) in the reference configuration is:

\[ \mathbf{v} = \frac{d\mathbf{x}}{dt} = \left. \frac{d\chi(\mathbf{x}, t)}{dt} \right|_{\mathbf{X}=\text{const.}} \quad (4) \]

The velocity gradient is now defined in the current configuration:

\[ \text{grad} \; \mathbf{v} = \mathbf{D} + \mathbf{W}, \quad (5) \]

where \( \mathbf{D} = \dot{\varepsilon} \) is the stretching rate (strain rate) and \( \mathbf{W} \) is the spin rate. It is assumed that the strain rate and the spin rate are uniform within each single crystal and denoted as \( \dot{\varepsilon}^c \) and \( \mathbf{W}^c \), respectively. The assumption comes from adopted homogenization procedure, discussed shortly.
The strain rate of a crystal can be additively decomposed:

\[ \dot{\varepsilon}^c = \dot{\varepsilon}^{el,c} + \dot{\varepsilon}^{pl,c}, \]  

(6)

where \( \dot{\varepsilon}^{el,c} \) is the elastic strain rate and \( \dot{\varepsilon}^{pl,c} \) is the plastic strain rate. The stress rate of the crystal is related to the elastic strain rate through Hooke’s law [14]:

\[ \dot{\sigma}^c = \mathbf{C}^c (\dot{\varepsilon}^c - \dot{\varepsilon}^{pl,c}) - \sigma^c tr(\dot{\varepsilon}^c), \]  

(7)

where \( \dot{\sigma}^c \) is the Jaumann rate of Cauchy stress and \( \mathbf{C}^c \) is an elastic stiffness tensor of a single crystal. Use of the objective Jaumann stress rate is necessary since due to action of spin, \( \mathbf{W}^c \), crystals will rotate during deformation. The relation (7) can be rewritten in linear form [14]:

\[ \dot{\sigma}^c = \mathbf{L}^c \dot{\varepsilon}^c, \]  

(8)

where \( \mathbf{L}^c \) is the elasto-plastic instantaneous stiffness tensor (or tangent stiffness). During the course of plastic deformation the \( \mathbf{L}^c \) will depend on the adopted evolution of the slip resistance, \( \tau^s_c \), with the shear strain on slip systems, \( \gamma^{s'} \):

\[ \tau^s_c = \tau^s_c(\gamma^{s'}), \]  

(9)

also referred to as the hardening law. Slip systems are defined by two directions: slip plane normal, \( \mathbf{n}^s \), and slip or burgers direction, \( \mathbf{b}^s \). Crystals deform plastically by shear on specific predetermined slip planes, \( \mathbf{n}^s \), in specific slip directions, \( \mathbf{b}^s \). More information about single crystal constitutive law can be found in Chapter 2, Section 2.1.
2.1.1.2 RVE constitutive law

Using the averaging procedure, Eq. (2), allows definition of the stress and strain rates in the RVE:

\[ \dot{\sigma} = \langle \dot{\sigma}^c \rangle \]  \hspace{1cm} (10)

\[ \dot{\varepsilon} = \langle \dot{\varepsilon}^c \rangle \]  \hspace{1cm} (11)

where \( \dot{\sigma} \) is the overall Jaumann rate and \( \dot{\varepsilon} \) is the overall strain rate. A linear form of the polycrystal constitutive relation is assumed [14]:

\[ \dot{\sigma} = L \dot{\varepsilon} \]  \hspace{1cm} (12)

where \( L \) is the effective tangent stiffness or the tangent stiffness of homogenous effective medium (HEM). The procedure for determination of \( L \) is referred to as homogenization. Based on the assumptions used to evaluate the stress in crystals, different homogenization procedures can be defined. In this work self-consistent homogenization is used. The crystals are assumed to be ellipsoidal heterogeneities in infinite matrix having the tangent stiffness of HEM, \( L \). Boundary conditions on the matrix are defined as either rate of traction or rate of displacement. Field equations to be satisfied in the matrix and heterogeneity are equilibrium, compatibility and constitutive relations for both matrix and the heterogeneity. Use of the Eshelby’s equivalent inclusion method allows solution of the boundary value problem and calculation of the stress and strain inside the heterogeneity, which come out to be uniform. Applying the Eshelby’s method and using the averaging procedure, Eqs. (10) and (11), allows calculation of \( L \) in terms of the single crystal tangent stiffness, \( L^c \), and the assumed
shape and orientation of ellipsoids representing crystals. More information about RVE constitutive law can be found in Chapter 2, Section 2.2.

2.1.2 Numerical integration

The presented rate equations define a continuum problem in the current configuration. The problem of the numerical integration can be formulated in the following way: an imposed strain rate to the RVE, \( \dot{\varepsilon} \), over a time increment, \( \Delta t \), is known, find the stress at the end of the time increment. In other words for the imposed strain history find the corresponding stress history [17]. The converged solution at time \( t \) is known. The goal of numerical integration is to transform the continuum set of rate equations into the set of incremental non-linear equations in fixed configuration, which can then be solved using standard methods for solution of non-linear equations.

During the increment in time, \( \Delta t \), crystals rotate due to the presence of the elastic spin [16]. Therefore, the continuum equations written at different instants in time are in different configurations. Summing the variables written in different configurations is not meaningful. Hence, all crystal variables are expressed in configuration at the beginning of the time increment using the incremental rotation matrix, \( \Delta \mathbf{R}^c(\tau) \), originating from the elastic spin of crystals [18]:

\[
\dot{\sigma}^c = \Delta \mathbf{R}^c(\tau) \dot{\sigma}^c \Delta \mathbf{R}^c(\tau); \quad \dot{\varepsilon}^c = \Delta \mathbf{R}^c(\tau) \dot{\varepsilon}^c \Delta \mathbf{R}^c(\tau),
\]

where the bar denotes that the variable is expressed in the configuration at the beginning of the time increment. Next, the single crystal constitutive law is integrated to the incremental form:

\[
\Delta \sigma^c = \mathbf{L}^{inc.c} \Delta \varepsilon^c,
\]

(14)
with:

\[ \bar{L}^{inc,c} = \frac{1}{\Delta t} \int_t^{t+\Delta t} \bar{L}^c dt, \]  

(15)

where \( \Delta \bar{\sigma}^c \) is the increment in stress, \( \Delta \bar{\varepsilon}^c \) is the increment in crystal strain and \( \bar{L}^{inc,c} \) is the incremental tangent stiffness. Likewise, the RVE constitutive relation is expressed in the incremental form:

\[ \Delta \bar{\sigma} = \bar{L}^{inc} \Delta \bar{\varepsilon} \]  

(16)

where \( \bar{L}^{inc} \) is the incremental HEM tangent stiffness. The incremental forms, Eq. (14) and Eq. (16), are plugged into the self-consistent homogenization, resulting in a system of non-linear equations in terms of the single crystal strain increments, \( \Delta \bar{\varepsilon}^c \). The system is solved using the Newton method. The detailed description of the implicit integration procedure can be found in Chapter 2, Section 3.

### 2.2 Coupling with finite elements

Finite element method statement of equilibrium condition at time \( t + \Delta t \) is:

\[ \mathbf{R}^{t+\Delta t}(\mathbf{u}^{t+\Delta t}) - \mathbf{F}^{t+\Delta t}(\mathbf{u}^{t+\Delta t}) = \mathbf{0}, \]  

(17)

where \( \mathbf{R} \) is the vector of externally applied nodal forces, \( \mathbf{u} \) is the vector of unknown nodal displacements and \( \mathbf{F} \) is the vector of internal forces calculated from element stresses as:

\[ \mathbf{F}^{t+\Delta t} = \sum_m \int_{V_m} \mathbf{B}^{m,T} \sigma^m dV \]  

(18)
where \( \mathbf{B} \) is an element strain-displacement matrix, \( \sigma \) is the stress within the element and \( m \) is the element number [19]. At instant in time \( t \) all variables are known and equilibrium is satisfied. The vector of nodal displacement can be written as:

\[
\mathbf{u}^{t+\Delta t} = \mathbf{u}^t + \Delta \mathbf{u},
\]

where \( \Delta \mathbf{u} \) is the unknown increment in nodal displacements. The iterations over increment in nodal displacements are performed until Eq. (17) is satisfied within a tolerance. For each iteration the numerical integration of Eq. (18) is performed and the integrand is evaluated at specific points in space i.e. integration points of the element. The constitutive relation is used to calculate the element stress at integration points at the end of the increment, \( \sigma_{FE}^{t+\Delta t} \), based on the guessed strain increment at the integration point, \( \Delta \varepsilon_{FE} \). The strain increment is formulated from guessed incremental displacement field, meaning that compatibility relations are satisfied. The incremental rotation matrix, \( \Delta \mathbf{R}_{FE} \), is also available to update the configuration.

Finite element software used in this study is Abaqus. Abaqus allows users to defined their own constitutive relation through user material subroutine (UMAT). The UMAT subroutine is called for each integration point for each guessed displacement field. The constitutive relation in this study is defined with elasto-plastic self-consistent (EPSC) model, hence the UMAT subroutine is necessary to interface between Abaqus and EPSC model.

The UMAT subroutine performs several steps. First, all tensors are rotated with \( \Delta \mathbf{R}_{FE} \) to update the configuration. Next, the guessed strain increment, \( \Delta \varepsilon_{FE} \), passed
from Abaqus is corrected and applied in numerical integration scheme presented in previous section. The correction of $\Delta \varepsilon_{FE}$ is introduced to enforce the equality:

$$\varepsilon_{FE}^{t+\Delta t} = \varepsilon_{FE}^t + \Delta \varepsilon_{FE} = \langle \varepsilon^{c,t+\Delta t} \rangle,$$  \hspace{1cm} (20)$$

where $\varepsilon_{FE}^t$ is the total strain at time $t$, calculated by Abaqus [20]. Disregarding the effect of crystal rotation in current increment allows straight forward calculation of the corrected strain increment:

$$\Delta \bar{\varepsilon} = \varepsilon_{FE}^t + \Delta \varepsilon_{FE} - \langle \bar{\varepsilon}^{c,t} \rangle.$$  \hspace{1cm} (21)$$

The corrected strain increment is applied in numerical integration procedure and $\Delta \bar{\sigma}$ is calculated as output and used to update the stress at the end of the time increment:

$$\sigma_{FE}^{t+\Delta t} = \langle \bar{\sigma}^{c,t} \rangle + \langle \Delta \bar{\sigma}^{c,t} \rangle = \langle \bar{\sigma}^{c,t} \rangle + \Delta \bar{\sigma}.$$  \hspace{1cm} (22)$$

Next, the derivative $\frac{\partial \Delta \sigma_{FE}}{\partial \Delta \varepsilon_{FE}}$ is calculated in order to obtain a new guess for incremental displacement field in non-linear analysis:

$$\frac{\partial \Delta \sigma_{FE}}{\partial \Delta \varepsilon_{FE}} = \frac{\partial (\sigma_{FE}^{t+\Delta t} - \sigma_{FE}^t)}{\partial \Delta \varepsilon_{FE}} = \frac{\partial \Delta \sigma}{\partial \Delta \varepsilon} = \frac{\partial (L \Delta \varepsilon)}{\partial \Delta \varepsilon} = L.$$  \hspace{1cm} (23)$$

Finally, the configuration with respect to the single crystal rotation is updated.

The presented stress update algorithm is developed for 3D stress elements and needs to be modified for use with other element types. Shell elements are often used in sheet metal forming due to their computational efficiency. At the integration points of shell elements plane stress state is assumed in plane of the sheet. Therefore, plane
stress state needs to be imposed in EPSC UMAT as well. The three updated components of stress corresponding to three corrected components of strain are:

\[
\begin{bmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{12}
\end{bmatrix}^{t+\Delta t} = \langle \begin{bmatrix}
\bar{\sigma}_{11} \\
\bar{\sigma}_{22} \\
\bar{\sigma}_{12}
\end{bmatrix}^{t} angle + \begin{bmatrix}
L_{11} & L_{12} & L_{16} \\
L_{21} & L_{22} & L_{26} \\
L_{61} & L_{62} & L_{66}
\end{bmatrix} - \begin{bmatrix}
L_{13} & L_{14} & L_{15} \\
L_{23} & L_{24} & L_{25} \\
L_{63} & L_{64} & L_{65}
\end{bmatrix} \begin{bmatrix}
L_{33} & L_{34} & L_{35} \\
L_{43} & L_{44} & L_{45} \\
L_{53} & L_{54} & L_{55}
\end{bmatrix}^{-1} \begin{bmatrix}
L_{31} & L_{32} & L_{36} \\
L_{41} & L_{42} & L_{46} \\
L_{51} & L_{52} & L_{56}
\end{bmatrix} \begin{bmatrix}
\Delta \bar{\varepsilon}_{11} \\
\Delta \bar{\varepsilon}_{22} \\
2\Delta \bar{\varepsilon}_{12}
\end{bmatrix} .
\] (24)

The Jacobian becomes a 3x3 matrix easily evaluated from Eq. (24). Derivation of relations used in the stress update algorithm and Jacobian matrix for 3D stress elements can be found in Chapter 2, Section 4, while the treatment of shell elements is presented in Chapter 3.

2.3 Material parameters calibration for polycrystal plasticity constitutive relation

The single crystal data needed for the model include:

1. Elastic stiffness of single crystal, \( C^c \)
2. Active deformation modes containing slip systems determined with burgers vector, \( b^s \), and slip plane normal vector, \( n^s \),
3. Hardening parameters determining evolution of slip resistance, \( \tau^s \), with accumulated shear strain, \( \gamma^s \),
4. Three Euler angles determining orientation of crystal frame with respect to a sample frame i.e. texture.
The first two sets of parameters are dependent on material in question and its crystal structure and can be found in literature. Hardening parameters define the behavior after onset of plasticity and are fitted based on the measured mechanical response of material being modeled. While all previous parameters are equal for all crystals, three Euler angles are different between crystals. The set of crystal orientations is determined from measured texture of material being modeled. Therefore, only hardening parameters need to be calibrated while the rest is either taken from literature or measured.

2.4 Validation

The validation of integration algorithm is performed with the explicit EPSC integration algorithm developed in [13, 14]. The elastic constants of Cu were used. Slip family \(\{111\}(1\bar{1}0)\) active in face centered cubic (FCC) materials was considered. Hardening law is defined with function \(\tau^s_c = \tau^s_c(y^s)\), provided in Chapter 2 with Eq. (56). The applied strain history is generated by applying 1000 strain increments:

\[
\Delta \varepsilon = \begin{bmatrix}
0.0003 & 0 & 0 \\
0 & -0.00015 & 0 \\
0 & 0 & -0.00015
\end{bmatrix}.
\] (25)

The initial texture is shown in Fig 1a. The deformed texture predicted by both implicit and explicit EPSC integration algorithms is shown in Fig 1b. The true stress vs true strain plot in direction 11 is compared in Fig 1c. The difference between generated stress histories by both integration algorithms is shown in Fig 1d. Additional validation of implicit integration algorithm and coupling with finite elements is provided in Chapter 2, Section 6.
Fig. 1. (a) \{002\} pole figure showing the initial set of crystal orientations used for the comparison study. Comparison of the predictions using the original explicit and the new implicit formulations after simple tension: (b) \{002\} pole figure showing the reoriented set of crystals, (c) true stress-true strain curves, and (d) the difference between stress histories produced by the models.

2.5 Computational time

The implicit algorithm developed here uses smaller number of sub-steps in the integration procedures than the original explicit formulation [13, 14], while achieving the same accuracy. The reduction of number of sub-steps in integration procedure should be reflected in the computational time. This is seen in Fig 2a where computational times for both explicit and implicit integration procedures are shown for varying number of sub-steps and level of accuracy. The comparison was performed for integration of strain history exported from Abaqus for one integration point of a shell element during the cup
drawing simulation. More information on the simulation set up and comparison is provided in Chapter 2, Section 6.2.1. Fig 2b shows the speed up in implicit code is for most part above 2, having a maximum of 8.56.

**Fig. 2.** (a) Computational time involved in the explicit and implicit integration procedures as a function of number of sub-steps. The number next to the explicit model points refers to the number of sub-steps in dividing the Abaqus strain increment, while the numbers next to the implicit model points refer to the number of sub-steps in dividing the Abaqus strain increment and the number of sub-steps used in the single crystal integration procedure, respectively. (b) Speed up of the implicit code relative to the explicit code for the same average error, calculated as the ratio of the explicit to the implicit computational times shown in (a).
3. Strain path sensitive hardening law for polycrystal plasticity: application to AA6022-T4

During a forming process each material point experiences a distinct strain path. Complex non-linear strain paths are routinely encountered in sheet metal forming processes [21]. In CBT simulation, frequent strain path reversals are encountered [8]. The strain path for a material point refers to collection of strain increments experienced by the material point during the forming process, i.e. strain history. Since plastic deformation is a path dependent process, the corresponding stress at any point on the strain path depends not only on the total value of strain, but also on the strain path to reach the total strain value [22]. With a change in the direction of strain increments transients are observed in the mechanical response [21, 23]. Therefore, the accuracy of the forming simulations and the CBT simulation is closely related to the capability of the constitutive law to capture the stress evolution during strain path changes.

The origin of macroscopically observed transients in mechanical response during strain path changes is found in microstructure evolution and development of residual stresses at different length scales. Dislocations are responsible for material behavior in plastic regime. Dislocations are line defects in crystal structure. Under the action of stress dislocations can move causing plastic shear strain on specific crystallographic planes, \( n^s \), in specific directions, \( b^s \). With increasing plastic strain average length of dislocation line per volume i.e. dislocation density, \( \rho \), increases. The increase in dislocation density is responsible for hardening observed after onset of plasticity. The evolution of dislocation density after strain path change is in part responsible for observed transients in mechanical response.
The objective of this section is to develop a polycrystal plasticity constitutive model accounting for transients in mechanical response observed during strain path changes. In the EPSC model the condition for onset of plastic shearing follows the Schmid law:

\[ \mathbf{\sigma}^c \cdot \mathbf{m}^s = \tau^s_c, \]  

(26)

where \( \mathbf{\sigma}^c \) is the stress in the crystal, \( \mathbf{m}^s = \frac{1}{2} (\mathbf{n}^s \otimes \mathbf{b}^s + \mathbf{b}^s \otimes \mathbf{n}^s) \) is the Schmid tensor and \( \tau^s_c \) is the slip resistance. The slip resistance is a function of dislocation density, while the dislocation density evolves with shear strain [24]. The EPSC model assumes the slip resistance evolves with shear strain:

\[ \dot{\tau}^s = \sum_{s'} h^{ss'} \dot{\gamma}^{s'}, \]  

(27)

where \( \dot{\gamma}^{s'} \) is the shear rate on slip system \( s' \) and \( h^{ss'} \) is the hardening matrix. In this work, it is assumed that the slip resistance can be expressed as a function of shear strain, Eq. (9). Therefore, the elements of the hardening matrix become partial derivatives: \( h^{ss'} = \frac{\partial \tau^s}{\partial \gamma^{s'}} \). The functional dependence of Eq. (9) is referred to as the hardening law. The residual stresses of type I (polycrystal level) and II (grain level) are intrinsically present in the EPSC model coupled with finite elements. The effect of type III (sub-grain level) residual stress are accounted for by addition of backstress to Eq. (26). More information on strain path sensitive hardening law formulation, implementation and calibration is provided in Chapters 4 and 5.

3.1 Dislocation based hardening law

The slip resistance is defined in terms of dislocation density [24]:

\[ \tau^s_c = f(\rho). \]
\[
\tau_s^c(\rho^s_{\text{tot}}, \rho_{\text{deb}}) = \tau_0^a + \tau_{\text{forest}}^s(\rho^s_{\text{tot}}) + \tau_{\text{deb}}^a(\rho_{\text{deb}})
\]

(28)

where \(\tau_0^a\) is an initial value that sums the contributions from the Peierls stress and Hall-Petch like term, \(\tau_{\text{forest}}^s\) stems from the statistically stored dislocation density \(\rho^s_{\text{tot}}\), \(\tau_{\text{deb}}^a\) comes from the amount of dislocations stored as substructure \(\rho_{\text{deb}}\). The functions \(\tau_{\text{forest}}^s(\rho^s_{\text{tot}})\) and \(\tau_{\text{deb}}^a(\rho_{\text{deb}})\) are defined in [24] together with functions \(\rho^s_{\text{tot}}(\gamma^s)\) and \(\rho_{\text{deb}}(\gamma^s)\). The incorporation of dislocation hardening law in explicit EPSC formulation [25] has been performed and applied to HCP Be [25]. The hardening matrix needed for coupling of hardening law with EPSC is:

\[
h_{ss'} = \frac{\partial \tau_{\text{forest}}^s}{\partial \rho^s_{\text{tot}}} \frac{\partial \rho^s_{\text{tot}}}{\partial y^{s'}} + \frac{\partial \tau_{\text{deb}}^a}{\partial \rho_{\text{deb}}(\gamma^s)} \frac{\partial \rho_{\text{deb}}(\gamma^s)}{\partial y^{s'}}.
\]

(29)

Next, extensions to the dislocation based hardening law accounting for mechanism related to strain path changes are proposed.

### 3.2 Backstress and dislocation based hardening law including latent hardening during strain path reversal

The forest contribution to the slip resistance in Eq. (28) follows the Taylor relation:

\[
\tau_{\text{forest}}^s = b^\alpha \chi \mu^\alpha \sqrt{\sum_{ss'} L^{ss'} \rho^s_{\text{tot}}} \rho_{\text{tot}}^{ss'}
\]

(30)

where \(b^\alpha\) is magnitude of the Burgers vector, \(\chi\) is an interaction constant, \(\rho^s_{\text{tot}}\) is the statistically stored dislocation density for \(s^{th}\) slip system belonging to \(\alpha\) slip mode \((s \in \alpha)\) and \(L^{ss'}\) is a strength interaction matrix [26]. The single crystal experiments and dislocation dynamics simulations show that off-diagonal terms of strength interaction matrix are larger than diagonal ones [27-32]. However, such strength interaction matrix
produces non-positive definite hardening matrix, $h^{ss'}$. Therefore, the necessary condition for determination of shear rates, $\dot{\gamma}$, on active slip systems is not fulfilled [33]. Issues in the solution procedure are encountered at the single crystal and polycrystal level due to the presence of such hardening matrices. The major issue is the loss of ellipticity of the polycrystal tangent stiffness. To circumvent the problem, hardening matrix, $h^{ss'}$, is corrected before evaluating the single crystal tangent stiffness, $L^c$. The corrected hardening matrix, $h^{ss'}_d$, is assumed to be diagonal, while it's elements are determined by the condition that both the original hardening matrix, $h^{ss'}$, and the corrected hardening matrix, $h^{ss'}_d$, produce the same rates in slip resistance:

$$\sum_{s't} h^{ss'}_{rs's'} \dot{\gamma}_{s'} = \sum_{s't} h^{ss'}_{rs's'} \dot{\gamma}_{s'},$$

(31)

where the indices $s$ and $s'$ go over active slip systems. Detailed discussion of the correction procedure and the effect of latent hardening on the mechanical response can be found in Chapter 5.

There have been many studies on the effect of strain path changes on the mechanical response [34-38]. The general conclusion is that the evolution of dislocation density $\rho_{for}^{s}(\gamma^s)$ appears to take a different form during strain path changes. In order to take into account the effect of strain history on the evolution of dislocation density, $\rho_{for}^{s}(\gamma^s)$ is split into two parts: forward dislocation density $\rho_{forw}^{s}(\gamma^s)$ and reversible dislocation density $\rho_{rev}^{s}(\gamma^s)$, which are evolved according to new laws proposed in [34, 39]. The implementation of the reversible dislocation model in the EPSC is described in Chapter 4, Section 3.1 and Chapter 5, Section 3.1.
Another phenomena important for response after strain path change is formation of internal stress field, termed backstress. The backstress field shows up due to formation of strain gradients inside crystals. After onset of plastic deformation dislocation structures form within crystals. For instance, crystals can become divided into soft cells, having low dislocation density, and hard cell walls, having high dislocation density [40]. The strain partitioning between cells and cell walls is such that cells accommodate more strain than cell walls due to difference in strength. The geometrically necessary dislocations (GNDs) show up due to presence of strain gradient. A dislocation is a defect in material giving rise to internal stress field. GNDs are ordered in such a way that stress fields from individual dislocations combine to produce long-range internal stress field, referred to as backstress. The backstress field will remain in the material after load is removed. Since the body is in equilibrium the backstress field should have zero volume average.

The backstress is included in the model by adding new terms in the activation conditions [41]:

\[ \sigma^c \cdot m^s - \tau_{bs}^s = \tau^s, \]  
\[ \dot{\sigma}^c \cdot m^s - \dot{\tau}_{bs}^s = \dot{\tau}^s, \]

where \( \tau_{bs}^s \) is the backstress on a slip system \( s \). The backstress is evolved in a similar way as the slip resistance:

\[ \dot{\tau}_{bs}^s = \sum_{s'} h_{bs}^{s's'} \dot{\gamma}^{s'}, \]
where $h_{ds}^{s'}$ is the backstress hardening matrix. Appropriate function to evolve the backstress with shear strain are based on previous works [23]. The details of backstress implementation in the EPSC can be found in Chapter 4, Section 3.2 and Chapter 5, Section 3.2.

**Fig. 3.** Comparison of measured (solid lines) and predicted (dashed lines): (a) true stress-true strain curves for simple tension in RD, TD and 45 directions, (b) corresponding r-ratio predictions and (c) large strain cyclic tension-compression response along RD for AA6022-T4.
The developed model was used to simulate plastic anisotropy in mechanical response and cyclic behavior of AA6022-T4. The obtained fits and predictions to experimental data are shown in Figure 3. The discussion of the effect of reversible dislocation evolution laws and backstress on predictions of mechanical response are provided in Chapter 4, Section 4.2, while the effect of the strength interaction matrix, $L^{ss'}$, is discussed in Chapter 5, Section 4.2.

4. Case study 1: Cup drawing of aluminum alloy AA6022-T4

In this section, the predictive capabilities of developed implicit EPSC model with strain path sensitive hardening law are demonstrated. The sheet metal forming process of cup drawing was simulated using Abaqus FE software coupled with EPSC UMAT subroutine. The material parameters of the model have been calibrated in Chapter 5, and the resulting fits to the experimental measurements of mechanical response are shown in Fig. 3 of previous section. The simulation set up is shown in Fig 4a. During the simulation the blank holder was fixed at constant distance from the die, while the punch was displaced downwards to draw the cup. Once the cup is fully formed contact between the cup and the die, the punch and the blank holder is removed to simulate the springback. The blank mesh is shown in Fig 4b. Details of the simulation set up and results are provided in Chapter 2, Section 6.2.
Fig. 4. Simulation setup: (a) deep drawing geometry and (b) FE quarter model of the initial blank containing 3950 shell elements. 79 elements are along the diameter and 50 elements are along the circumference of the blank.

The results of the simulation in terms of contours of von Mises stress after forming and after springback are shown in Fig 5a and b, while the formed cup geometry is presented in Fig 5c. Due to the presence of texture in the material the stress distribution and the cup shape are not axisymmetric. From the simulation results following information are available: the shape of the formed cup, residual stress distribution at two length scales (type I and type II residual stress distribution), texture evolution, slip system activity. More information on the cup drawing simulation can be found in Chapter 2, Section 6.2.2 and Chapter 3, Section 4. Furthermore, the deformed cup shape can be compared with experimental measurements.
Fig. 5. Deformed mesh with contours of von Mises stress (a) after forming and (b) after springback. (c) Deformed mesh after springback.
5. Case study 2: Polycrystal plasticity modeling of mechanical fields and microstructure evolution during simple tension and CBT of AA6022-T4

Bending under tension, as a stabilizing mechanism related to incremental sheet forming (ISF), can be studied by means of the CBT test. The finite element CBT test simulation set up is shown in Fig 6, while the experimental set up is shown in Fig 7. A constant crosshead velocity is applied to the right end of the specimen in Fig 6, while the left end is fixed. The three rollers travel along the gauge length of the specimen, superimposing bending stresses to tensile stresses induced by applied crosshead velocity. The material of the specimen is aluminum alloy AA6022-T4.

The modeling framework for mechanical response of AA6022-T4 during strain path changes was summarized in previous sections. The strain paths experienced by material points close to the surface of the specimen contain multiple strain path reversals induced by the passage of rollers. Cyclic plasticity experiments, reproducing such complex strain paths, were performed on aluminum alloy AA6022-T4 at Tokyo University of Agriculture & Technology [42]. The cyclic plasticity experiments were used
to calibrate the hardening parameters of the developed EPSC model. The calibrated EPSC model is then used to define the constitutive relation in the finite element model of the CBT test. The predictions of the force-displacement profile during the CBT test and the texture evolution are shown in Fig 8a and b. The model is able to reproduce the experimental trends in force-displacement behavior and texture evolution during the CBT test. More information on the calibration of the EPSC model and finite element simulation of the CBT process is available in Chapter 6, Sections 2 and 3, respectively.

Fig. 7. Experimental set up for CBT test [5].
Fig. 8. (a) The measured and simulated force displacement profile during the CBT test. (b) The measured texture after 12 CBT cycles and the simulated texture after 8.5 CBT cycles.

From post-processing of the CBT simulation results it is concluded that at each instant in time only regions in proximity of rollers experience plastic deformation. Due to the asymmetric loading conditions along the through thickness direction, a gradient in axial plastic strain along the through thickness direction is observed. Comparison of
state variables at the same level of axial plastic strain between the CBT processed material and the simple tension (ST) does not show significant differences. Only minor differences are noticed, in particular, the state after the CBT appears to have: (1) more uniform plastic strain distribution over grains, (2) higher average dislocation density and (3) slower crystal reorientation. More information on the mechanical response during CBT test and comparison between the CBT and ST can be found in Chapter 6, Section 4.

References


CHAPTER 2:

An implicit formulation of the elasto-plastic self-consistent polycrystal plasticity model and its implementation in implicit finite elements

This chapter is a preprint of a paper submitted for publication in Mechanics of Materials Journal as: "An implicit formulation of the elasto-plastic self-consistent polycrystal plasticity model and its implementation in implicit finite elements", Milovan Zecevic and Marko Knezevic. The research and writing of this chapter was performed in typical student-advisor relationship.
An implicit formulation of the elasto-plastic self-consistent polycrystal plasticity model and its implementation in implicit finite elements

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Abstract

Elasto-plastic self-consistent (EPSC) polycrystal plasticity theory has been used extensively in understanding and predicting anisotropic thermo-mechanical response and underlying microstructure evolution of polycrystalline metals. This paper describes the first implicit formulation of the EPSC model and its implementation in implicit finite elements. To this end, a suitably defined system of non-linear equations at the single crystal level and that at the polycrystal level homogenizing the single crystal solutions in terms of the rotation-neutralized increments in Cauchy stress and strain are formulated and numerically solved. The implicit EPSC model is first validated using the original explicit EPSC model. Subsequently, the implicit EPSC model is coupled with implicit finite elements (FE) through the use of the user material subroutine in Abaqus. To facilitate the efficient coupling, a stress update algorithm is developed and the consistent tangent stiffness operator is analytically derived. Here, every FE integration
point embeds the implicit EPSC constitutive law taking into account microstructure evolution and the directionality of deformation mechanisms acting at the single crystal level. The multi-level FE-EPSC model is benchmarked using the single crystal data for copper and then applied to simulate drawing of a cup from an AA6022-T4 sheet. The implementation and insights from these predictions are presented and discussed in this paper.

*Keywords*: Polycrystalline material; Crystal plasticity; Numerical algorithms; Finite elements; Deep drawing
1. Introduction

Metallic materials undergoing shaping and forming operations experience large plastic strains as well as frequent unloading and reloading, which cause highly non-uniform spatial stress-strain fields [1-3]. It is well known that crystallographic slip accommodates most of the plastic strains, while inducing plastic anisotropy in the mechanical response by evolution of crystallographic texture and dislocation structure. Additionally, intra- and inter-granular mechanical fields develop playing an important role in the deformation process, especially during unloading and reloading [4-6]. Upon a strain path change, the material exhibits non-linear unloading [2] followed by a reduction in yield stress from that reached at the end of pre-loading. The phenomenon is referred to as the Bauschinger effect (BE) [4]. The hardening rate that follows with continuation of loading is also different from that during pre-loading [7, 8]. These characteristics of material behavior are governed by the evolution of the underlying microstructure and crystallographic texture. Crystal plasticity constitutive theories are designed to capture the underlying physics governing such microstructure evolution and the associated anisotropic stress-strain response of polycrystalline metals.

Over the past several decades, a number of crystal plasticity based models have been developed. For example, these include upper bound Taylor-type models [9, 10] and mean-field self-consistent models [11-14]. As stand-alone (SA) codes, these models facilitate monotonic deformation, while not accounting for the heterogeneities in the mechanical fields that develop across the sample as a consequence of complex geometry and/or strain path changes during metal forming. In contrast, crystal plasticity finite element (CPFE) and crystal plasticity fast Fourier transform (CPFFT) models can
calculate the spatially resolved mechanical fields over explicit grain structure in 3D [15-20]. However, these spatial models are computationally intensive and are typically used for modeling a representative volume element of a given material rather than a forming process. As a compromise, the mean-field models have been integrated in finite elements to operate at FE integration points facilitating complex deformation paths [21-25].

One of the mean-field formulations is the elasto-plastic self-consistent (EPSC) model [14]. It is desirable because it accounts for granular elasticity. The model has been shown capable of predicting residual stress fields, elastic lattice strains, non-linear unloading, the BE, and hardening rates along with texture and twinning for various metals in a number of studies [26-30]. The strategy of embedding the EPSC model at the meso-scale level in an implicit FE analysis at the macro-level was described in [31] for continuum elements and in [32] for shell elements. The overall model was termed FE-EPSC. The tangent stiffness matrix (Jacobian) required for the coupling was derived analytically facilitating fast convergence towards stress equilibrium.

In EPSC, the integration scheme for the rate equations is explicit. Specifically, the single crystal stress and shearing rates as well as the single crystal tangent stiffness are evaluated at the beginning of the given time increment and, thus, the self-consistent homogenization for the macroscopic tangent stiffness is performed with crystal properties evaluated at the beginning of the time increment [14, 30]. Due to the explicit integration, the magnitudes of strain and rotation increments are limited to rather small values. The original FE-EPSC incorporating the explicit EPSC model required a sub-stepping procedure for strain increments passed from Abaqus to ensure accuracy of
simulations [31]. Such small values of increments can lead to a significant increase in the computational time due to the need to solve many increments. Computational efficiency is particularly a concern for the FE-EPSC implementation. In any simulation of a forming operation on polycrystalline metals using FE-EPSC, the single crystal stress equations for a large number of constituent grains followed by the self-consistent homogenization need to be solved at every integration point in the FE mesh for every trial displacement field. The time involved in the calculations scales approximately linearly with the number of increments. Thus, the main motivation of the development of the implicit EPSC model is to enable the FE-EPSC model to facilitate the use of large strain increments and eventually utilize strain increments provided by Abaqus relaxing the need for any sub-stepping. In addition, the lack of convergence of fixed-point iterations for calculation of polycrystal tangent stiffness occasionally occurs in cases when the number of constituent crystals used is small (on the order of a hundred), which is again the case relevant for FE-EPSC, where we attempt to minimize the amount of state variables and computational time. FE-EPSC typically runs with a hundred or a few hundred weighted orientations at each integration point.

To improve the efficiency of the original explicit EPSC formulation, this paper describes an implicit formulation of the EPSC model and its implementation in implicit finite elements. To this end, a suitably defined system of non-linear equations, homogenizing the single crystal solutions in terms of the rotation-neutralized increments in Cauchy stress and strain, is created and solved using Newton’s method. The implicit EPSC model is first validated using the original explicit EPSC model. Case studies demonstrate that the implicit implementation can take large strain and rotation
increments. Subsequently, the implicit EPSC mode is coupled with implicit finite elements using the user material subroutine in Abaqus. The consistent tangent stiffness operator is analytically derived to provide the so-called Jacobian for the FE residual iterations. To illustrate the potential of the coupled multi-level FE-EPSC model, a sheet metal forming process of deep drawing subjecting the material to a multi-axial deformation path is simulated. A cup is drawn of an Al alloy AA6022-T4 sheet. In addition to drawing, the subsequent springback unloading step is simulated. Here, granular elasticity, intra-granular backstresses, backstress aided dislocation glide, and inter-granular stresses are taken into account. Shell elements are used in the simulation as sheet metal forming simulations are typically performed using shell elements because of their computational efficiency. The FE-EPSC multi-level model developed in this work can be used as a simulation tool for simulating forming of anisotropic metals taking into account the effects of microstructure on the flow properties.

2. Constitutive relations

In the presence of large strains and rotations, a constitutive relation between the Jaumann rate of Cauchy stress, $\dot{\sigma}$, and the average strain rate, $\dot{\varepsilon}$, for a material point is [30, 33]:

$$\dot{\sigma} = L \dot{\varepsilon} = \dot{\sigma} + \sigma W - W \sigma,$$

(1)

where $L$ is the tangent stiffness, $\sigma$ is the Cauchy stress, and $W$ is the spin tensor. The relation holds for a material point, which could be thought as the representative volume element (RVE) of the material i.e. a minimum volume of the material such that the response from the volume is representative for the continuum [34]. The material point
can be a single crystal or a polycrystalline point. While single crystals are usually assumed to be homogenous, polycrystalline materials are heterogeneous because they consist of single crystals, which introduces heterogeneities in the mechanical fields. Thus, defining constitutive relation for a polycrystalline material involves a homogenization of known responses of constituent single crystals. In what follows, a brief review of generally accepted relations describing constitutive response of polycrystalline metallic materials is given [14, 30, 33, 35-38]. In our description, “·” and “⊗” are used to denote a dot product and a tensor product, respectively.

2.1 Single crystal constitutive relation

Every single crystal occupies some volume in a polycrystal. During a deformation process, every point in this volume experiences motion. The strain rate and spin rate kinematic quantities are calculated from the motion. The quantities are assumed to be uniform within each single crystal and are denoted as $\dot{\varepsilon}^c$ and $W^c$, respectively. Since the material time derivative for velocity is from the current position vector, $\dot{\varepsilon}^c$ and $W^c$ are expressed in the current configuration. All relations in this section are likewise written with respect to the current configuration.

Hooke’s law, in the rate form, for a crystal undergoing rigid body rotation, in the presence of plastic strain, is:

$$\dot{\sigma}^c = C^c (\dot{\varepsilon}^c - \dot{\varepsilon}^{pl,c}) - \sigma^c tr(\dot{\varepsilon}^c),$$  \hspace{1cm} (2)

where $\dot{\sigma}^c$ is the Jaumann rate of Cauchy stress, $C^c$ is an elastic stiffness tensor of a single crystal, $\dot{\varepsilon}^c$ is a total strain rate and $\dot{\varepsilon}^{pl,c}$ is a plastic strain rate. The plastic strain rate inside crystal is defined as:
\[ \varepsilon^{pl,c} = \sum_s m^s \dot{\gamma}^s, \]  

(3)

where \( m^s = \frac{1}{2} (b^s \otimes n^s + n^s \otimes b^s) \) is the symmetric Schmid tensor, defined by \( b^s \), which is the slip system Burgers vector in the current configuration and \( n^s \), which is the slip system normal vector in the current configuration. \( \dot{\gamma}^s \) is a shear rate on the slip system \( s \). The sum is over all active slip systems. Slip systems are active if they fulfill the following conditions:

\[ \sigma^c \cdot m^s = \tau^s_c, \]  

(4a)

\[ \bar{\sigma}^c \cdot m^s = \dot{\tau}^s_c, \]  

(4b)

where \( \tau^s_c \) is the slip resistance of a slip system \( s \). The values of slip resistance per \( s \) define the single crystal yield surface. The first condition means that for a slip system to be active, the stress state needs to be on the yield surface, while the second condition is the consistency condition, which ensures that the stress state remains on the yield surface. The yield surface evolves due to strain hardening. The evolution of slip resistance is coupled with shearing rates using:

\[ \dot{\tau}^s_c = \sum_{s'} h^{s's'} \dot{\gamma}^{s'}, \]  

(5)

where \( h^{s's'} \) is the hardening matrix. It is assumed that the evolution of slip resistance is a known function of shear strain, \( \tau^s_c(\gamma^{s'}) \). As a result, the hardening matrix is a matrix of partial derivatives \( h^{s's'} = \frac{\partial \tau^s_c}{\partial \gamma^{s'}}(\gamma^{s''}) \). Specific expressions for the evolution of slip resistance and the hardening matrix are described later. Following Eq. (1), the single crystal constitutive relation is:
\[ \ddot{\varepsilon}^c = \mathbf{L}^c \dot{\varepsilon}^c . \] (6)

In Eq. (6), \( \mathbf{L}^c \) is the elasto-plastic instantaneous stiffness tensor (or the tangent stiffness) and is given by [30]:

\[ \mathbf{L}^c = \mathbf{C}^c - \mathbf{C}^c \sum_s \mathbf{m}^s \otimes \left( \sum_{s'} (X^{ss'})^{-1} \mathbf{m}^{s'} (\mathbf{C}^c - \sigma^c \otimes \mathbf{i}) \right) - \sigma^c \otimes \mathbf{i} , \] (7)

with:

\[ X^{ss'} = h^{ss'} + \mathbf{C}^c \cdot \mathbf{m}^s \otimes \mathbf{m}^{s'}, \] (8)

where \( \mathbf{i} \) is the second rank identity tensor, and indices \( s \) and \( s' \) span over all active slip systems in a grain \( c \). The tangent stiffness in the elasto-plastic deformation regime has the same meaning as the elastic stiffness in the elastic deformation regime, with that it applies to the rates of stress and strain and not the total quantities, and therefore can be referred to as the property of a single crystal.

It remains to define the crystal rigid body rotation for crystal reorientation i.e. texture evolution. The elastic spin rate of a crystal \( c \) is:

\[ \mathbf{W}^c = \mathbf{W}^{c,\text{app}} - \mathbf{W}^{\text{pl},c} , \] (9)

where \( \mathbf{W}^{c,\text{app}} \) is a total applied spin and \( \mathbf{W}^{\text{pl},c} \) is a plastic spin. This total applied spin is a sum of an overall applied macroscopic spin, \( \mathbf{W} \), and a spin originating from the antisymmetric Eshelby tensor for crystal \( c \), \( \mathbf{\Pi}^c \), which will be defined shortly. The plastic spin is:

\[ \mathbf{W}^{\text{pl},c} = \sum_s \dot{\gamma}^s \mathbf{q}^s , \] (10)
where $q^s = \frac{1}{2}(b^s \otimes n^s - n^s \otimes b^s)$ is the antisymmetric Schmid tensor.

### 2.2 Polycrystalline constitutive relation

The polycrystalline constitutive relation used in the present work is that of the EPSC model [39]. This model relates the deformation of each crystal to the deformation of the polycrystal using the self-consistent homogenization scheme [14, 30]. The polycrystal is represented by a collection of single crystals each having a specific crystal lattice orientation, an ellipsoidal shape, and a volume fraction. The mechanical fields of each crystal are determined by considering each crystal as an elasto-plastic inclusion in the homogeneous equivalent medium (HEM). The HEM has properties of the polycrystal, which is assumed to be an RVE of a material.

Homogeneous boundary conditions are treatable by a standalone EPSC (SA-EPSC) model. For example, we can impose strain increments ($\varepsilon \Delta t$) along the loading direction, while enforcing zero average stress along the two lateral directions of the sample to simulate simple tension/compression. An applied deformation can consist of an applied spin, $W$, like in simple shear deformation. In contrast to SA-EPSC, FE-EPSC can handle any boundary conditions facilitated by the FE framework, as will be described later.

Following Eq. (1), the linear constitutive relation between the Jaumann rate of Cauchy stress and the strain rate for a polycrystal is:

$$\dot{\sigma} = L \dot{\varepsilon}$$ \hspace{1cm} (11)
where $\dot{\sigma}$ is the overall Jaumann rate, $\dot{\varepsilon}$ is the overall strain rate, and $L$ is the tangent stiffness of HEM i.e. the polycrystal. The HEM tangent stiffness is defined based on the self-consistent homogenization approach. The unknown tangent stiffness of the HEM can be determined by enforcing:

$$\dot{\sigma} = \langle \dot{\sigma}^c \rangle,$$
$$\dot{\varepsilon} = \langle \dot{\varepsilon}^c \rangle,$$

(12)
(13)

where $\langle \rangle$ indicate volume average over single crystal quantities, $c$. The above relations result in an implicit equation for the HEM tangent stiffness:

$$L = \langle L^c A^c \rangle \langle A^c \rangle^{-1},$$

(14)

with:

$$A^c = (L^c + L^*)^{-1}(L + L^*),$$
$$L^* = L(S^c^{-1} - I),$$

(15)
(16)

where $L$, $L^c$, $L^*$ and $S^c$ are the macroscopic tangent stiffness, the crystal tangent stiffness, an interaction tensor, and the symmetric portion of the Eshelby tensor, respectively.

From the Eshelby solution of a single crystal inhomogeneity inside HEM and applied boundary conditions, an additional spin per crystal is calculated as:

$$\Pi^c = P^c(S^c)^{-1}(\dot{\varepsilon}^c - \dot{\varepsilon}),$$

(17)

where $P^c$ is the antisymmetric Eshelby tensor and $\Pi^c$ is the calculated spin.
3. Implicit integration of the rate equations in EPSC

The rate equations presented in section 2 describe a continuum problem in the current configuration. An imposed strain rate, \( \dot{\varepsilon} \), and a spin rate, \( \mathbf{W} \), to a polycrystal are known. These constitute an applied strain history. The objective is to find the stress history using an integration algorithm [40]. The converged solution at time \( t \) is known and the integration is performed over a time increment \( \Delta t \). The imposed deformation, \( \dot{\varepsilon} \), and the rigid body rotation, \( \mathbf{W} \), can be treated separately [41]. The decoupling allows separate treatment of any imposed rigid body rotation by simply rotating all tensors with an incremental rotation matrix, \( \Delta \mathbf{R} \), which corresponds to \( \mathbf{W} \). Therefore, the macroscopic spin is not explicitly needed for the integration procedure and, thus, is not considered to act in the rate equations presented in section 2. The single crystal constitutive equation, Eq. (2), is integrated to incremental form [33]. The integration requires a choice of a fixed configuration in which variables are expressed and integrated. Likewise, the polycrystal constitutive equation needs to be expressed in an incremental form at a fixed configuration. Once the equations are in the incremental form, in a given configuration, the problem can be formulated as a set of non-linear equations. As a result, the continuum model is replaced with a nonlinear incremental model [40]. Several steps are specifically identified in the integration algorithm developed in the present work: (a) decoupling deformation and rotation, (b) integrating the single crystal constitutive relation, and (c) solving a system of non-linear equations for a polycrystal in an incremental form.

It is worth mentioning that the integration of a single crystal response can be treated independently from the polycrystal homogenization procedure [42]. Several
single crystal algorithms have been proposed in literature [37, 43-46]. The integration algorithm followed in the present work was proposed as explicit in [43], but first introduced in [47]. The algorithm was further developed as implicit in [45]. The algorithm is particularly suitable for the present development because it solves for the time increment over which there is no change in active slip systems, for the known set of active slip systems at the start of the increment. On the other hand, other evaluated algorithms use fixed time increment and search for the unknown set of active slip systems. This results in a situation that a set of active slip systems is essentially enforced to be active during the whole time increment, creating a strong constraint which cannot always be successfully satisfied, especially if time increments are large. The solution procedure for the system of non-linear equations at a polycrystal level follows the procedure developed for the visco-plastic self-consistent (VPSC) model in [11], with some adjustment.

3.1 Decoupling deformation and rotation effects at a single crystal level

Generally, a crystal is simultaneously subjected to a strain rate, $\dot{\varepsilon}^c$, and a spin rate, $W^c$. Even though the macroscopic spin is not considered, there are still the plastic spin, $W^{pl,c}$, and the spin from antisymmetric Eshelby tensor, $\Pi^c$, contributing to $W^c$. We distinguish three configurations: the initial configuration for the current increment at $t$, the current configuration at $\tau$ ($t < \tau < t + \Delta t$), and the configuration at the end of the current increment $t + \Delta t$. Figure 1 shows the configuration at $t$ and the configuration at $t + \Delta t$ for a crystal with respect to the sample frame. We remind that the continuum rate equations presented in section 2 are intrinsically expressed in the current configuration, $\tau$. 

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Integration of a tensor must be performed in one configuration, since addition of tensors defined in different configurations is not meaningful. Therefore, one configuration needs to be chosen and all tensors should be rotated to this configuration before integration. We choose the known configuration at \( t \) to express all tensor quantities [33]. The rotation tensor that rotates vectors from the configuration at \( t \) to the current configuration at \( \tau \) is:

\[
\mathbf{n}^c = \Delta \mathbf{R}^c(\tau) \mathbf{n}^c, \tag{18}
\]

where \( \mathbf{n}^c \) is a vector in the configuration at \( t \), \( \mathbf{n}^c \) is a vector in the configuration at \( \tau \) and \( \Delta \mathbf{R}^c(\tau) \) is an incremental active rotation matrix calculated from the spin, \( \mathbf{W}^c \). Next, we can rotate all essential quantities to the configuration at \( t \) using [33]:

\[
\bar{\mathbf{\sigma}}^c = \Delta \mathbf{R}^c(T)\mathbf{\sigma}^c \Delta \mathbf{R}^c(\tau) \; ; \; \bar{\mathbf{\dot{\sigma}}}^c = \Delta \mathbf{R}^c(T)\mathbf{\dot{\sigma}}^c \Delta \mathbf{R}^c(\tau) \; ; \; \bar{\mathbf{\mathbf{W}}}^c = \Delta \mathbf{R}^c(T)\mathbf{W}^c \Delta \mathbf{R}^c(\tau) \; ; \; \bar{\mathbf{\mathbf{\dot{W}}}^c} = \Delta \mathbf{R}^c(T)\mathbf{\dot{W}}^c \Delta \mathbf{R}^c(\tau) \; \; ; \; \bar{\mathbf{\varepsilon}}^c = \Delta \mathbf{R}^c(T)\mathbf{\varepsilon}^c \Delta \mathbf{R}^c(\tau) \; ; \; \bar{\mathbf{L}}^{ijkl} = \Delta \mathbf{R}_{pi}(\tau)\Delta \mathbf{R}_{qj}(\tau)\Delta \mathbf{R}_{rk}(\tau)\Delta \mathbf{R}_{sl}(\tau)\mathbf{L}_{pqrs}. \tag{19}
\]

Quantities expressed in the configuration at \( t \) are called the rotation-neutralized quantities and are denoted with the bar on top of them. The constitutive relation expressed in terms of the rotation-neutralized quantities is:

\[
\bar{\mathbf{\dot{\sigma}}}^c = \bar{\mathbf{L}}^c \bar{\mathbf{\mathbf{\varepsilon}}}^c, \text{ with the initial condition of } \bar{\mathbf{\sigma}}^c(t) = \bar{\mathbf{\sigma}}^c_0. \tag{20}
\]

If we integrate the Eq. (20), we obtain the increment in stress [33]:

\[
\Delta \bar{\mathbf{\sigma}}^c = \int_t^{t+\Delta t} \bar{\mathbf{L}}^c \bar{\mathbf{\mathbf{\varepsilon}}}^c dt = \frac{1}{\Delta t} \left( \int_t^{t+\Delta t} \bar{\mathbf{L}}^c dt \right) \Delta \bar{\mathbf{\mathbf{\varepsilon}}}^c, \tag{21}
\]
where $\dot{\varepsilon}^c = \frac{\Delta \varepsilon^c}{\Delta t} = \text{const}$. This amounts to applying the deformation defined with $\Delta \bar{\varepsilon}^c$, followed by the rotation $\Delta R^c_{t+\Delta t} = \Delta R^c(t = t + \Delta t)$ of all tensors to configuration at $t + \Delta t$, as shown in Figure 1. For instance, the stress is updated using:

$$\sigma^c_{t+\Delta t} = \Delta R^c_{t+\Delta t}(\bar{\sigma}^c_t + \Delta \bar{\sigma}^c)\Delta R^c_{t+\Delta t}^T. \tag{22}$$

![Diagram showing configurations at $t$ and $t + \Delta t$](image)

**Fig. 1.** Configurations at $t$ and $t + \Delta t$ showing decoupling of deformation, $\dot{\varepsilon}^c$, and rotation corresponding to $W^c$.

### 3.2 Integration of the single crystal constitutive relation in its incremental form

The incremental form of the constitutive law for a single crystal is:

$$\Delta \bar{\sigma}^c = \overline{L}^{inc,c} \Delta \bar{\varepsilon}^c, \tag{23}$$

where $\overline{L}^{inc,c} = \frac{1}{\Delta t} \int_t^{t+\Delta t} \overline{L}^c dt$ is the tangent stiffness relating the increments in strain and Cauchy stress. We conveniently introduce the new variable, $\overline{L}^{inc,c}$, for the integral of $\overline{L}^c$ since the latter might be evaluated multiple times within the increment. Examination of the expression for tangent stiffness (7) and (8) shows the dependence:
\[ \mathbf{L}^c = \mathbf{L}^c(A, \mathbf{\bar{\sigma}}^c, h^{ss'}) \], with \( s, s' \in A(\mathbf{\bar{\sigma}}^c, h^{ss'}, \mathbf{\bar{\tau}}^s, \mathbf{\bar{\epsilon}}^c) \),

where \( A \) is a set of active slip systems and \( s \) and \( s' \) go over active slip systems belonging to \( A \). It is important to note that the set of active slip systems is determined based on the activation conditions (4a and b). Note also that for all active slip systems the condition, \( \dot{\gamma}^s > 0 \), must be fulfilled.

We point out that sub-discretization of a time increment \( \Delta t \) is a characteristic of our integration scheme. As a result, \( \Delta t \) can be reduced to \( \Delta t_{sub} \) in two ways. First, the sub-increment, \( \Delta t_{sub} \), can be specified as an input and used throughout a simulation. Second, \( \Delta t \) can be reduced to \( \Delta t_{sub} \) by the integration procedure, as will be discussed below. Here, the sub-increment, \( \Delta t_{sub} \), is treated as an unknown in the integration procedure.

If sub-discretization is not set up as the input, the rule is that the integration algorithm updates variables from the start of the increment, \( t \), to the end of the increment \( t + \Delta t \). The exception is if the sub-discretization of the time increment is triggered then \( t_{sub} \) is initialized to \( t \) and then updated incrementally for \( \Delta t_{sub} \) until the end of the increment \( t + \Delta t \).

A set of potentially active slip systems is determined with Eq. (4a) written at the \( t \). A system of linear equations in terms of the unknown shear rates, \( \dot{\gamma}^{s'}_t \), can be suitably formed using the consistency condition, Eq. (4b), along with Eqs. (2), (3) and (5) expressed at \( t \):

\[
\left( \mathbf{\bar{C}}^c \mathbf{\bar{\epsilon}}^c - \mathbf{\bar{\sigma}}^c tr(\mathbf{\bar{\epsilon}}^c) \right) \cdot \mathbf{\bar{m}}^s = \sum_{s'} (h^{ss'}_t + \mathbf{\bar{C}}^c \cdot \mathbf{\bar{m}}^{s'} \otimes \mathbf{\bar{m}}^s) \dot{\gamma}^{s'}_t ,
\] (25)
with $\dot{\varepsilon}^c = \frac{\Delta \varepsilon^c}{\Delta t}$ and $\dot{\gamma}^s' = \frac{\Delta \gamma^s'}{\Delta t}$. Knowing the shear rates, $\dot{\gamma}^s'$, the remaining single crystal quantities can be readily evaluated. Since the variables used in solving for the shear rates, $\dot{\gamma}^s'$, are all at $t$, the algorithm is explicit. If a shear rate is negative for some of the active slip systems, they are removed from the set of active slip systems and Eq. (25) is reevaluated for the set of modified shear rates. This algorithm has been used in the standard EPSC model.

In our development, we formulate an implicit solution procedure for shear rates facilitating large time increments. To this end, Eq. (25) can be written at a time instant anywhere after $t$ up to and including $t + \Delta t$. We conveniently chose to write it at the mid instant, i.e. $t + \frac{\Delta t}{2} = t_m$:

$$
\left( \bar{C}^c \dot{\varepsilon}^c - \bar{\sigma}^{c*}_{\text{r}} + \bar{C}^c \cdot \bar{m}^s \otimes \bar{m}^s \right) \cdot \bar{m}^s = \sum_{s'} (h^{s's'}_{\text{r}} + \bar{C}^c \cdot \bar{m}^{s'} \otimes \bar{m}^s) \dot{\gamma}^{s'}_{\text{r}}.
$$

(26)

Now, Eq. (26) represents a system of non-linear equations in terms of $\dot{\gamma}^{s'}_{\text{r}}$, since the hardening matrix, $h^{s's'}_{\text{r}}$, and the stress, $\bar{\sigma}^{c*}_{\text{r}}$, depend on shear rates. Since Eq. (26) is satisfied at an instant of time after $t$, the integration is implicit.

As always, the stress state at the end of the increment needs to be on or within the single crystal yield surface. The condition is enforced with Eq. (26) for all active slip systems, and any shift in inactive slip systems must be checked:

$$
\bar{\sigma}^{c*}_{\text{r}+\Delta t} \cdot \bar{m}^s \leq \tau^{s'}_{\text{c},\text{r}+\Delta t},
$$

(27)

with:
\[
\bar{\sigma}_{t+\Delta t}^c = \bar{\sigma}_t^c + \Delta t \dot{\bar{\sigma}}_{t_m}^c,
\]
\[
\tau_{c,t+\Delta t}^s = \tau_{c,t}^s + \Delta t \sum s' h_{s'}^{t_m} \dot{\gamma}_{s'}^{t_m}.
\]

If the condition is violated for any of the inactive slip systems, meaning they become active during the increment, the increment \( \Delta t \) is adjusted so that only one of the inactive slip systems satisfies [43]:

\[
\bar{\sigma}_{t+\Delta t}^c \cdot \bar{m}^s = \tau_{c,t+\Delta t}^s.
\]

As a result, the increment is reduced to the maximum value before activating the additional slip system, while the stress remains on the crystal yield surface. Equation (30) is an additional relation to the system in Eq. (26) formulated to calculate \( \Delta t_{sub} \) [43, 45] as:

\[
\Delta t_{sub} = \min \frac{\tau_{c,t}^s - \bar{\sigma}_t^c \cdot \bar{m}^s - \sum s' h_{s'}^{t_m} \dot{\gamma}_{s'}^{t_m}}{\bar{\sigma}_m^c \cdot \bar{m}^s - \sum s' h_{s'}^{t_m} \dot{\gamma}_{s'}^{t_m}},
\]

where \( \min \) takes the minimum calculated value out of all inactive slip systems.

Analogues to \( t_m \), the mid instant becomes \( t_{sub,m} = t_{sub} + \frac{\Delta t_{sub}}{2} \). The sub-increment, \( \Delta t_{sub} \), is often calculated in the elasto-plastic transition and in any strain path change portion of deformation but rarely otherwise. We use the fixed point iteration scheme to solve the formulated system of non-linear equations for shear rates, \( \dot{\gamma}^s \), and \( \Delta t_{sub} \). If there is no activation of any new slip systems within the increment then the solution for \( \Delta t_{sub} \) is \( \Delta t \).

In summary, the procedure for \( i^{th} \) iteration consists of the following steps:
1. Determine the set of potentially active slip systems, \( A_t \), using the condition in Eq. (4a) written at \( t \):

\[
\bar{\sigma}_t^c \cdot \bar{m}^c = \tau_c^S. \tag{32}
\]

2. Evaluate the hardening matrix, \( \hat{h}_{im}^{s'} \), and the stress, \( \bar{\sigma}_m^c \), at the time instant

\[
t_m = t + \frac{\Delta t^i}{2}
\]

using the guessed shear rates \( \dot{\gamma}_{im}^{s',i} \) for the increment \( \Delta t^i \).

3. Calculate the shear rates, \( \dot{\gamma}_{im}^{s',i+1} \), from the system of linear equations, i.e. Eq. (26). If any of the calculated shear rates is negative, the corresponding active slip system is removed from the set of potentially active systems, \( A_t \), and the system of linear equations is solved again for the set of shear rates corresponding to the corrected set of active slip systems.

4. Find the tangent stiffness at instant \( t_m \) and update the stress increment using:

\[
\bar{L}_m^c = \bar{L}^c(A_t, \bar{\sigma}_m^c, \hat{h}_{im}^{s'}) \tag{33}
\]

\[
\Delta \bar{\sigma}^c = \frac{\partial \bar{L}^c}{\partial t} \Delta t^i. \tag{34}
\]

5. Evaluate Eq. (31) to determine if a new slip system activated during the increment and calculate the sub-increment, \( \Delta t_{sub}^{i+1} \), over which the determined set of active slip systems remains constant. Any of slip systems removed in step 3, due to occurrence of their negative shear rate, are not considered.

6. Check for convergence by comparing increments in shear strain:
\[
\sqrt{\sum_{i} \left( \dot{\gamma}_{tm}^{i} \Delta t^{i+1} - \dot{\gamma}_{tm}^{i} \Delta t^{i} \right)^2} < 0.005. \tag{35}
\]

If condition (35) is not fulfilled return to step 1.

Upon convergence, if the stress exited the single crystal yield surface because of the slip systems removal in step 3, the slip resistances are corrected so that the stress is on the single crystal yield surface:

\[
\tau_{c,t+\Delta t}^s = (\bar{\sigma}_t^c + \Delta \bar{\sigma}^c) \cdot \bar{m}^s. \tag{36}
\]

Next, \( \bar{L}^{inc,c} \) can be calculated. If the sub-incremental procedure is triggered then, \( \bar{L}^c \) is evaluated at multiple instances, \( k \), during the total time increment, \( \Delta t \). Here, the incremental tangent stiffness is a sum of those at the instances, \( k \):

\[
\bar{L}^{inc,c} = \frac{1}{\Delta t} \int_{t+\Delta t}^{t} \bar{L}^c dt = \frac{1}{\Delta t} \sum_{k} \bar{L}^c_{t_{sub,m}} \Delta t_{sub,m}^k. \tag{37}
\]

Note that the incremental tangent stiffness, \( \bar{L}^{inc,c} \), is evaluated with, \( \bar{L}^c_{t_{sub,m}} \), at \( t < \tau < t + \Delta t \), and not from \( t \). The subsequently calculated polycrystal tangent stiffness, \( \bar{L}^{inc} \), will contain information at \( t < \tau < t + \Delta t \), making the overall procedure implicit.

Finally, the incremental plastic spin is evaluated using Eq. (10) as:

\[
\bar{W}^{pl,c} \Delta t = \sum_{k} \bar{W}_{t_{sub,m}}^{pl,c} \Delta t_{sub,m}^k = \sum_{s} \sum_{k} \dot{\gamma}_{t_{sub,m}}^s \bar{q}^s \Delta t_{sub,m}^k. \tag{38}
\]

In closing this section, we point out that the calculation of \( \Delta t_{sub} \) is an important addition to the single crystal integration procedure in EPSC. A vector representing the current stress in stress space can easily exit the yield surface if a constant increment size is
used like in the standard explicit EPSC, since the set of active slip systems at $t$ is assumed to be active during the increment. Furthermore, if the stress vector at time $t$ is within the single crystal yield surface, the response is assumed to be elastic during the increment, regardless whether the updated stress at $t + \Delta t$ is out of the yield surface. Equation (31) allows the calculation of the portion of the increment over which the set of slip systems does not change. Subsequently, only this portion of the sub-increment is applied. The algorithm prevents the stress from exiting the single crystal yield surface regardless of the size of the sub-increment specified.

3.3 Solution procedure for a system of non-linear equations at the polycrystal level in an incremental form

The polycrystal incremental form of the constitutive law is obtained by performing the self-consistent homogenization of the incremental single crystal constitutive law solutions. This amounts to replacing the Jaumann rate of Cauchy stress and strain rate with the rotation-neutralized increment in Cauchy stress and the rotation-neutralized increment in strain, respectively. The term rotation-neutralized quantities at the polycrystal level is used to denote that the rotation-neutralized quantities at the single crystal level are used in deriving the macroscopic response. The macroscopic response is:

$$\Delta \bar{\sigma} = \bar{L}^{inc} \Delta \bar{\varepsilon},$$

(39)

where $\bar{L}^{inc}$ is the HEM tangent stiffness, (Eq. (14)).

Replacing the rate form of the single crystal constitutive relation (Eq. (6)) and the polycrystal constitutive relation (Eq. (11)) in the homogenization procedure with their
incremental forms (i.e. Eq. (23) and Eq. (39)), produces a system of non-linear equations. The unknown variable in the system is the crystal strain increment $\Delta \bar{\varepsilon}^c$, since the proposed algorithm for single crystal integration is strain driven.

Next, we suitably define a residual in terms of $\Delta \bar{\varepsilon}^c$. For an initial guess of the $\Delta \bar{\varepsilon}^c$ field, the single crystal integration can be performed to obtain an increment in stress $\Delta \bar{\sigma}_{int}^c = \bar{L}_{inc,c}^c \Delta \bar{\varepsilon}^c$ and the tangent stiffness $\bar{L}_{inc,c}^c$. This is depicted in Fig. 2a, where a crystal is shown independently, outside of the matrix, under the strain increment $\Delta \bar{\varepsilon}^c$. Based on the calculated stress increment, $\Delta \bar{\sigma}_{int}^c$, we can find the traction on the surface of the ellipsoid needed to produce the applied strain increment:

$$
\Delta \bar{t}_{int}^c = \Delta \bar{\sigma}_{int}^c \bar{n}^c,
$$

where $\Delta \bar{t}_{int}^c$ is an increment in traction on the surface and $\bar{n}^c$ is a normal to the surface. The same is done for every crystals $c$. Based on the calculated tangent stiffness, $\bar{L}_{inc,c}^c$, the overall stiffness of polycrystal, $\bar{L}_{inc}^c$, can be calculated using Eq. (14). Next, we consider the matrix having the tangent stiffness of the HEM, $\bar{L}_{inc}^c$, from which the crystal $c$ was removed to apply the strain increment, $\Delta \bar{\varepsilon}^c$, to it (Fig. 2b). Now, the matrix has a cavity undergoing the increment in strain, $\Delta \bar{\varepsilon}^c$, which is needed to fit the inhomogeneity back in it. The matrix has a certain displacement increment applied at its boundary giving rise to the strain and stress increments. The traction on the surface of the cavity, needed to produce the strain increment, $\Delta \bar{\varepsilon}^c$, can be calculated from the interaction equation:

$$
\Delta \bar{\sigma}_{ext}^c = \Delta \bar{\sigma} - \bar{L}^* (\Delta \bar{\varepsilon}^c - \Delta \bar{\varepsilon}),
$$

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where $\Delta \sigma^c_{ext}$ is the external stress increment giving rise to the traction increment $\Delta \tau^c_{ext}$:

$$\Delta \tau^c_{ext} = \Delta \sigma^c_{ext}(-\mathbf{n}^e).$$

(42)

In order to satisfy the equilibrium when the inclusion is placed back inside the matrix, the external and internal tractions must be in balance:

$$\Delta \tau^c_{int} + \Delta \tau^c_{ext} = \Delta \sigma^c_{int} \mathbf{n}^e + \Delta \sigma^c_{ext}(-\mathbf{n}^e) = 0,$$

(43)

which leads to:

$$\Delta \sigma^c_{ext} - \Delta \sigma^c_{int} = 0.$$  

(44)

The balance between the external and internal stress increments is used to define the following residual:

$$r(\Delta \varepsilon^c) = \Delta \sigma^c_{ext} - \Delta \sigma^c_{int} = \Delta \bar{\sigma} - \mathbf{L}^\ast(\Delta \varepsilon^c - \Delta \varepsilon) - \mathbf{L}^c \Delta \varepsilon^c.$$  

(45)

The residual indicates how well the interaction equation is satisfied. As mentioned earlier, the definition of the residual along with the solution procedure were inspired by the algorithm present in VPSC [11]. In VPSC, the fixed point iterations are used for the evaluation of crystal stress. For each iteration, an appropriate interaction equation, analogous to Eq. (45), is solved in order to produce a new guess for crystal stress.

Finally, Newton's method is used to obtain the solution $\Delta \varepsilon^c$ by minimizing the residual. The Jacobian needed for Newton's method is defined as:

$$J^c = \frac{\partial r(\Delta \varepsilon^c)}{\partial \Delta \varepsilon^c} \approx -\mathbf{L}^\ast - \mathbf{L}^c.$$  

(46)
To test for convergence, the volume average of residuals for all grains is calculated and compared against the tolerance, i.e.:

\[
\frac{10^k(t(\Delta \epsilon^c))}{\|\Delta \sigma\|_{\text{avg}}} < 0.005.
\] (47)

with:

\[
\|\Delta \sigma\|_{\text{avg}} = \frac{\sum_{i=1}^{n_{inc}} \|\Delta \sigma^i\| \Delta t^i}{t}
\] (48)

where \(n_{inc}\) is the number of time increments applied by the time \(t\) i.e. \(t = \sum_{i=1}^{n_{inc}} \Delta t^i\) and \(k \geq 0\) is the smallest integer fulfilling the condition \(0.1 < \|\Delta \sigma\|_{\text{avg}}/(10^k \|\Delta \sigma\|) < 10\). If convergence is not achieved within predefined number of iterations the full Newton step is sequentially decreased with factors of 0.5, 0.2 and 0.1. If the condition (47) is still not satisfied after decreasing the Newton step, the applied increment in strain is applied within 4 steps, while the exponent \(k\) in the convergence criteria (47) is not reevaluated. The same procedure is used if one of the sub-increments is not converging. The cutting of strain increment and normalization of residual are inspired by the procedures used in Abaqus [41]. Once the criterion in Eq. (47) is fulfilled for the total imposed strain increment or all sub-increments, crystal spin, \(\vec{W}^c \Delta t\), can be updated and the corresponding rotation matrices, \(\Delta \mathbf{R}^c_{t+\Delta t}\), can be calculated. The plastic spin was calculated during integration of the single crystal constitutive law in section 3.1 (Eq. (37)). Since the macroscopic spin is not present, the only remaining spin is coming from the deviation of the single crystal strain rate from the applied macroscopic strain rate, due to treatment of single crystals as ellipsoidal inclusions in an infinite medium. This
contribution to the total crystal spin is described by Eq. (17). The total incremental elastic spin is:

$$\mathbf{W}^c \Delta t = \mathbf{\Pi}^c \Delta t - \mathbf{W}^{pl,c} \Delta t$$  \hspace{1cm} (49)

The incremental rotation matrix for single crystal, $\Delta \mathbf{R}^c_{t+\Delta t}$, is calculated from incremental spin defined with Eq. (49). With $\Delta \mathbf{R}^c_{t+\Delta t}$ all variables are rotated to the configuration at the end of the increment, $t + \Delta t$.

**Fig. 2.** Schematic showing the definition of the residual in terms of: (a) internal and (b) external stress increment.

4. **Coupling of the implicit EPSC model with implicit finite elements**

The coupling is performed with Abaqus through a user material subroutine (UMAT). It is important to note that Abaqus relies on the current configuration to
express all tensors and vectors. The current configuration is formed by applying the rigid body rotation to the known configuration at \( t \) [41]. In the description that follows, we will use the subscript \( FE \) to denote variables used in the communication with the FE software.

The constitutive relation within finite elements is used to calculate stress at the end of the increment, \( \sigma_{FE}^{t+\Delta t} \), based on the guessed total strain increment, \( \Delta \varepsilon_{FE} \), which results from the applied boundary conditions over the FE model. The incremental rotation matrix, \( \Delta R_{FE} \), is also provided in UMAT by Abaqus to update the configuration. The algorithm for stress update inside UMAT is as follows:

1. All tensors in EPSC including crystal orientations are rotated to the configuration at \( t + \Delta t \) with \( \Delta R_{FE} \) incremental rotation matrix for consistency with variables from Abaqus, since Abaqus rotates them to \( t + \Delta t \) before passing them to UMAT. With respect to the imposed macroscopic rotation the configuration is \( t + \Delta t \). However, the single crystal rotation due to the applied strain increment from Abaqus is unknown beforehand. Therefore, all crystal quantities will be kept at \( t \) with respect to the single crystal rotation.

2. Total strain at a material point at the end of the time increment is:

\[
\varepsilon_{FE}^{t+\Delta t} = \varepsilon_{FE}^t + \Delta \varepsilon_{FE}.
\] (50)

where \( \varepsilon_{FE}^{t+\Delta t} \), \( \varepsilon_{FE}^t \), and \( \Delta \varepsilon_{FE} \) are the total strain at the end of the time increment, the strain at the beginning of the increment, and the strain increment, respectively. The total strain at the end of the time increment corresponds to the total strain accommodated by the HEM material point at the end of the time increment, while the total stress returned to
the Abaqus corresponds to the stress in the HEM. Therefore, the following conditions are valid:

\[
\begin{align*}
\varepsilon_{FE}^{t+\Delta t} &= \varepsilon_{FE}^t + \Delta \varepsilon_{FE} = \langle \varepsilon^{c,t+\Delta t} \rangle = \langle \Delta R_{t+\Delta t}^c (\tilde{\varepsilon}^{c,t} + \Delta \tilde{\varepsilon}^c) \Delta R_{t+\Delta t}^c \rangle^T \\
\sigma_{FE}^{t+\Delta t} &= \langle \sigma^{c,t+\Delta t} \rangle = \langle \Delta R_{t+\Delta t}^c (\tilde{\sigma}^{c,t} + \Delta \tilde{\sigma}^c) \Delta R_{t+\Delta t}^c \rangle^T
\end{align*}
\]

(51a) (51b)

In Eq. (51a) the strain at the beginning of the time increment, \(\tilde{\varepsilon}^{c,t}\), and the total strain from the FE software, \(\varepsilon_{FE}^{t+\Delta t}\), are known. The crystal strain increment, \(\Delta \tilde{\varepsilon}^c\), stress increment, \(\Delta \tilde{\sigma}^c\), and incremental rotation matrix, \(\Delta R_{t+\Delta t}^c\), are calculated by performing the numerical integration described in section 3 under the imposed strain increment, \(\Delta \tilde{\varepsilon}\). Note that the single crystal strain increment, \(\Delta \tilde{\varepsilon}^c\), can be expressed in terms of the applied polycrystalline strain increment, \(\Delta \tilde{\varepsilon}\), using the localization tensor, \(\tilde{A}^c\), defined with Eq. (15), as: \(\Delta \tilde{\varepsilon}^c = \tilde{A}^c \Delta \tilde{\varepsilon}\). Also, the incremental rotation matrix, \(\Delta R_{t+\Delta t}^c\), is calculated from the total incremental spin, \(\tilde{W}^c \Delta t\), defined with Eq. (49), where \(\tilde{W}^c \Delta t\) is dependent on the imposed strain increment \(\Delta \tilde{\varepsilon}\). In presence of crystal rotations, the imposed strain increment, \(\Delta \tilde{\varepsilon}\), satisfying the Eq. (51a), is not equal to \(\Delta \varepsilon_{FE}\). This is clearly seen by looking at the first strain increment \(\Delta \varepsilon_{FE}\). Imposing the increment \(\Delta \varepsilon_{FE}\) in the integration procedure enforces Eq. (13) in the incremental form: \(\Delta \varepsilon_{FE} = \langle \Delta \tilde{\varepsilon}^c \rangle\). Once the update due to crystal rotation is performed the equality no longer holds: \(\Delta \varepsilon_{FE} \neq \langle \Delta R_{t+\Delta t}^c \Delta \tilde{\varepsilon}^c \Delta R_{t+\Delta t}^c \rangle^T\).

However, if an appropriate strain increment \(\Delta \tilde{\varepsilon}\) is applied instead of \(\Delta \varepsilon_{FE}\) the condition \(\Delta \varepsilon_{FE} = \langle \Delta R_{t+\Delta t}^c \tilde{A}^c \Delta \tilde{\varepsilon} \Delta R_{t+\Delta t}^c \rangle^T\) can be satisfied. Similar analysis can be performed for any subsequent increment. Therefore, equation (51a) represents a set of 6 non-linear equations in terms of the unknown imposed strain increment, \(\Delta \tilde{\varepsilon}\). Solving Eq. (51a) for \(\Delta \tilde{\varepsilon}\) involves an iterative procedure, in which for each iteration a new guess for \(\Delta \tilde{\varepsilon}\) is
made. For each guess for $\Delta \varepsilon$, the integration procedure (section 3) is performed. Since the integration procedure is where majority of time is spent in UMAT, the simulation time is increased significantly with each new guess for $\Delta \varepsilon$. To avoid the expensive iterations, the Eq. (51a) is rewritten, neglecting the effect of crystal rotations within current increment i.e. $\Delta \mathbf{R}_{t+\Delta t}^c$ is set to identity:

$$
\varepsilon_{FE}^t + \Delta \varepsilon_{FE} = \langle \varepsilon_c^{c.t} \rangle + \langle \Delta \varepsilon_c^{c} \rangle.
$$

(52)

Using Eq. (13), enforced by the homogenization procedure in the incremental form, allows for a straightforward calculation of the imposed strain increment from Eq. (52):

$$
\Delta \varepsilon = \varepsilon_{FE}^t + \Delta \varepsilon_{FE} - \langle \varepsilon_c^{c.t} \rangle.
$$

(53)

(3) Numerical integration described in section 3 is performed with imposed strain increment defined with Eq. (53). The integration can be performed with the calculated increment in strain from Eq. (53), or any sub-increments of $\Delta \varepsilon$, if the macroscopic sub-incrementation is chosen.

(4) Using the same approach for Eq. (51b) as for Eq. (51a) allows the calculation of stress at the end of the time increment:

$$
\sigma_{FE}^{t+\Delta t} = \langle \sigma_c^{c.t} \rangle + \langle \Delta \sigma_c^{c.t} \rangle = \langle \sigma_c^{c.t} \rangle + \Delta \sigma
$$

(54)

(5) All tensors referring to crystal frames are rotated for the crystal incremental rotation matrix, $\Delta \mathbf{R}_{t+\Delta t}^c$, calculated from spin acting over increment in time $\Delta t$ using Eq. (49). In other words, the configuration with respect to single crystal rotation is updated to $t + \Delta t$ at the very end of the procedure.
In addition to the stress update procedure, the Jacobian, \( \frac{\partial \Delta \sigma_{FE}}{\partial \Delta \epsilon_{FE}} \), needs to be calculated in order to obtain a new guess for the incremental displacement field in the non-linear implicit FE analysis. The derivative is:

\[
\frac{\partial \Delta \sigma_{FE}}{\partial \Delta \epsilon_{FE}} = \frac{\partial \left( \sigma_{FE}^{t+\Delta t} - \sigma_{FE}^{t} \right)}{\partial \Delta \epsilon_{FE}} = \frac{\partial \Delta \sigma}{\partial \Delta \epsilon} = \mathbf{L}
\]

The bars denote that all quantities, including the Jacobian, are evaluated consistently with Eqs. (53) and (54) in the configuration at \( t \) with respect to the single crystal rotation. It should be noted that the analytical evaluation of the Jacobian presented here is much more elegant than that presented in the original FE-EPSC implementation [31] because the rotation and deformation effects are decomposed and single crystal rotation during the current time increment is filtered when the stress at the end of the time increment is updated with Eq. (54). In [31] several sub-steps were used and configuration was updated after each sub-step, resulting in complicated dependence of the increment in stress on the applied strain increment. It should be noted that the developed stress update procedure and the Jacobian calculation are independent on the integration algorithm and can be used both with the original explicit and with the newly developed implicit integration. The difference between use of the implicit integration vs. the explicit integration is only present in step 3 of the stress update procedure.

In the implicit implementation the sub-steps are not necessary because the implicit implementation can handle large increments. The increments driven by Abaqus can be used, while the original explicit EPSC implementation in implicit finite elements relied on a sub-stepping algorithm. It was possible to use increments driven by Abaqus in the original implementation but the calculations were inaccurate, which is the intrinsic
limitation of any explicit solution procedure. Therefore, in the current study, we have simplified the Jacobian, ensured the accurate solution with large increments with no need for sub-stepping of those passed by Abaqus, and as a result gained the computational efficiency.

5. Validation of the implicit polycrystal integration algorithm

The implicit EPSC model is first validated using the explicit EPSC model in terms of true stress-true strain response and the evolution of crystal reorientation. For the comparison purpose, a simple hardening law involving three fitting parameters is implemented in both codes:

\[
\tau_c^s = \tau_0 + \sum_{s'} L^{ss'} Q \left(1 - \exp(-b \gamma_{s'})\right),
\]

where \(Q = 40\) and \(b = 10\) are fitting parameters and \(\tau_0 = 50\) MPa is the initial slip resistance. Only self-hardening is allowed by setting the strength interaction matrix to \(L^{ss} = 1\) and \(L^{ss'} = 0\). The hardening law enters the EPSC model through the hardening matrix used in Eq. (5). Since an expression for the evolution of slip resistance in function of shear strain on slip system is adopted, elements of the hardening matrix are partial derivatives of slip resistance with respect to the shear strain on the slip system:

\[
h^{ss'} = \frac{\partial \tau_c^s}{\partial \gamma_{s'}} = L^{ss'} b Q \exp(-b \gamma_{s'}) .
\]

The modeling framework and integration algorithm are general and can handle any hardening law. The material is Cu. The elastic constants of Cu are \(C_{11} = 170\) GPa, \(C_{12} = 124\) GPa and \(C_{44} = 75\) GPa [44]. The slip family \(\{111\}\{1\bar{1}0\}\), active in face centered cubic (FCC) materials, was considered. 10 orientations shown in Fig. 3a were used as the initial texture. Uniaxial tension in 1000 strain increments has been imposed using:
\[
\Delta \varepsilon = \begin{bmatrix}
0.0003 & 0 & 0 \\
0 & -0.00015 & 0 \\
0 & 0 & -0.00015 \\
\end{bmatrix}.
\] (57)

In the explicit code, for each imposed strain increment, 150 equal sub-increments were used to integrate the constitutive relation ensuring absence of any appreciable error in the simulation. In order to have a fair comparison between the explicit and implicit EPSC models, the explicit EPSC model follows the same procedure for stress updated to the one described in section 4 with a difference that the explicit integration is used in step 3. The number of sub-increments was determined by performing a sub-increment sensitivity study, in which the number of sub-increments was increased until the results stopped changing. In contrast, no sub-incrementation was specified as an input for the integration of single crystal constitutive law in the implicit code. A more detail analysis of the effect of sub-increment size in explicit and implicit integration algorithms will be presented in section 6.2.1 on a more involved case study in finite elements. The comparison of the predicted textures and true stress in the direction 11 and true strain in the direction 11 at the end of the simulation is shown in Fig. 3b and c. The relative difference between stress histories is shown in Fig 3d. The relative difference between stress histories is below 0.2 %, confirming that both integration methods produce similar results. Some possible contributions to the difference between the results are identified next. The solution procedure in the explicit and implicit EPSC is different. In the implicit EPSC the strain increments of single crystals are varied until the residual defined in terms of the single crystal stress increments is below prescribed tolerance. On the other hand, in explicit EPSC the homogenized tangent stiffness is varied using the fixed point
Fig. 3. (a) \{002\} pole figure showing the initial set of crystal orientations used for the comparison study. Comparison of the predictions using the original explicit and the new implicit formulations after simple tension: (b) \{002\} pole figure showing the reoriented set of crystals, (c) true stress-true strain curves, and (d) the difference between stress histories produced by the models.

iterations until difference between the new guess and the previous guess for the homogenized tangent stiffness is lower than a prescribed tolerance. Due to differences in the solution procedures, the calculated single crystal variables and the homogenized tangent stiffness are not the same between the explicit and implicit integration schemes, even when the tolerances are decreased to very small values for very fine increments.
Another source of the difference is the intrinsic sub-incrementation of the single crystal response within the implicit code upon activating an additional slip system, preventing the stress from exiting the single crystal yield surface. In the standard EPSC there is no such mechanism, and exit of stress out of the single crystal yield surface is inevitable when slip systems are first activated. The problem can be circumvented by using large number of sub-steps, which was done here.

6. Simulations using FE-EPSC

In this section, the multi-level FE-EPSC model incorporating the implicit EPSC is benchmarked using the single crystal data for Cu and then applied to simulate drawing of a cup from an aluminum alloy AA6022-T4 sheet.

6.1 Benchmark case study: Single crystals

Single crystal tension simulations without hardening performed in [44] are used to validate the single crystal integration algorithm and texture update algorithm. One brick continuum finite element with 8 nodes and 8 integration points in three-dimensional space (labeled as C3D8 in Abaqus convention) is used. The model is set consistent with the simulation setup presented in [44]. The slip systems belonging to \(\{111\}\langle1\bar{1}0\rangle\) family are allowed to activate. The entries of the hardening matrix are set to sufficiently small values, \(h_{ss'} = 0.01\). The results of simulations for three different crystal orientations are shown in Fig. 4. As expected, the orientations [001] and [1\(\bar{1}\)1] are stable, while [2\(\bar{3}\)6] is not stable but evolves. The results show good match between the approach presented here and the one used in [44]. Some differences in the rate of crystal reorientation and stress level are seen for the tension of [2\(\bar{3}\)6] orientation. We
attribute the mismatch to the difference in the formulation used here and that used in [44]. The major source of mismatch is the assumed update of plastic deformation gradient given with relation (50) in [44]:

$$\mathbf{F}_{t+\Delta t}^P = (\mathbf{I} + \sum_s \Delta \gamma^s \text{sign}(\tau^s_t)\mathbf{b}^s_t \otimes \mathbf{n}^s_t)\mathbf{F}_t^P,$$  \hspace{1cm} (58)

where $\mathbf{F}^P$ is plastic deformation gradient. Enforcing small time increments, we can assume $\Delta \gamma^s \ll 1$ and $\Delta \gamma^s \Delta \gamma^{s'} \approx 0$. Expanding the relation for $n$ number of steps and disregarding higher order terms in $\Delta \gamma^s$:

$$\mathbf{F}_n^P = \mathbf{I} + \sum_i \sum_s \Delta \gamma^s_i \text{sign}(\tau^s_i)\mathbf{b}^s_i \otimes \mathbf{n}^s_i.$$  \hspace{1cm} (59)

The actual plastic deformation gradient after $n$ steps is:

$$\mathbf{F}_n^P = \mathbf{I} + \sum_i \sum_s \Delta \gamma^s_i \text{sign}(\tau^s_i)\mathbf{b}^s_n \otimes \mathbf{n}^s_n.$$  \hspace{1cm} (60)

Incremental update of plastic deformation gradient does not account for the contribution coming from the rotation of crystal with accumulated shear strain on slip systems. To verify that this effect is indeed the source of the difference we compare the results of tension of $\{\overline{2}36\}$ orientation from [44] with two modeling approaches within implicit EPSC model. The first approach relies on the strain increment correction procedure in section 4. The method corrects the applied strain increment from Abaqus with a "strain increment" originating from an additional single crystal rotation of the total strain in the crystal. The additional rotation is present due to the plastic spin. The model predicts slightly higher stress and more rapid reorientation of single crystal orientation as can be seen in Fig. 4c. The second modeling approach neglects the effect of plastic spin on rotation of total strain tensor and simply applies the total strain increment from Abaqus.
The comparison with the first modeling method and the result from [44] is shown in Fig. 4c. Both the stress strain response and the crystal reorientation are closer to those presented in [44].

Fig. 4. Comparison of the predicted crystal lattice reorientation and true stress-true strain response under simple tension for three single crystals. The loading axis relative to the crystal frame is indicated for each single crystal.
6.2 Application case study: Deep drawing of AA6022-T4

In this section the implicit integration procedure is used in conjunction with an advanced dislocation density-based hardening law considering the kinematic backstress effects. The hardening model has been calibrated to predict anisotropic mechanical response during monotonic loading as well as linear and non-linear unloading, the Bauschinger effect and hardening rates upon the load reversal for AA6022-T4. Most generically, it accounts for the development of intra-granular backstresses, backstress aided dislocation glide, thermally activated storage of dislocations, elastic anisotropy, inter-granular stresses, and crystallographic slip. The law is summarized in the appendix A. Tables 1 and 2 show the material parameters. These were calibrated using the explicit EPSC model in an earlier study [39] and used here in the implicit EPSC model. Figure 5 shows the comparison between measured and calculated results for the monotonic tension in RD, 45°, and TD, corresponding r-values, and the cyclic response in RD. The anisotropy in the simulated flow curves, seen in Figure 5a, was attributed to an accurate latent hardening description with the experimentally evaluated strength interaction matrix, $L$, [48]. While the flow curves were used for fitting the hardening law material parameters, the r-values, shown in Figure 5b, are predictions, which are not very sensitive to the hardening law fitting parameters. The backstress fitting parameters and the reversible dislocations parameters, described in appendix A, were fit by comparing the simulated and the measured cyclic response in RD, shown in Figure 5c. The model slightly over-predicts the amount of permanent softening i.e. the drop in the stress level during the compression in comparison to the initial tension. A possible cause of the discrepancy between the simulated and measured cyclic curves is
Fig. 5. (a) Measured texture of AA6022-T4 sheet. Comparison between measured and simulated mechanical response of AA6022-T4: (b) monotonic true stress-true strain curves along the three loading directions as indicated in the legend, (c) evolution of r-ratio along the same three loading directions as in (b), and (d) cyclic response along RD to different amounts of pre-strain as indicated in the legend.
the over-predicted inter-granular residual stress. The EPSC formulation is closer to the Taylor iso-strain than to the Sachs iso-stress homogenization assumption [39]. The inter-granular residual stresses are large in the Taylor homogenization, while the Sachs homogenization does not predict the appearance of inter-granular residual stresses. The inter-granular residual stresses are known to influence the cyclic behavior of materials [49-51]. It is worth pointing out that the same calculation results can be obtained using the standard explicit EPSC.

Table 1. Constitutive parameters for the evolution of slip resistance for {111}(110) slip mode in AA6022-T4.

<table>
<thead>
<tr>
<th>$L^s_{copolanar}$</th>
<th>$L^s_{non-coplanar}$</th>
<th>$g^s$</th>
<th>$g^{ss'}$</th>
<th>$\tau_0$[MPa]</th>
<th>$k_1$[m$^{-1}$]</th>
<th>$g$</th>
<th>$D$[MPa]</th>
<th>$q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>1.4</td>
<td>1</td>
<td>1</td>
<td>56</td>
<td>0.65 x10$^8$</td>
<td>0.0294</td>
<td>100</td>
<td>8</td>
</tr>
</tbody>
</table>

Table 2. Parameters for the evolution of slip system kinematic backstress in AA6022-T4.

<table>
<thead>
<tr>
<th>$\tau_{bs}^{sat}$[MPa]</th>
<th>$v$</th>
<th>$\gamma_b$</th>
<th>$A$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>560</td>
<td>0.001</td>
<td>10</td>
</tr>
</tbody>
</table>

The simulation results in Fig. 5 are shown for 219 orientations representing the ODF reconstructed from an EBSD scan. Since the run time of any EPSC simulation is proportional to the number of crystals used, the ODF is represented with a minimum number of orientations that still give representative mechanical response of the material based on the procedure described in [52, 53].

Figure 6 shows the deep drawing simulation set up and the blank mesh [32]. The set up consists of a die, a blank holder, and a punch. The friction coefficient is set to 0.1. The punch, the die, and the blank holder are modeled as analytical rigid surfaces.
The blank thickness is 1.2 mm, which is modeled with 5 integration points through the thickness. During the simulation blank holder is held fixed at 1.2 mm from the die, while the punch is displaced downwards in order to draw the cup. After drawing, the contact between the drawn cup, punch, die and blank holder is removed in order to simulate springback. Only one quarter of the cup was modeled due to the orthotropic texture (Fig. 5a). The blank mesh size was determined based on a mesh-sensitivity study. Three mesh sizes were tested: coarse (25 S3R and 975 S4R shell elements), medium (50 S3R and 3900 S4R shell elements) and fine (100 S3R and 15600 S4R shell elements). The medium mesh is shown in fig 6b. \( J_2 \) material behavior i.e. the von Mises yield surface, was used for mesh sensitivity study. The yield stress in function of the equivalent plastic strain was entered in a tabular form to reproduce the simple tension.
true stress-true strain curve in the RD. The medium mesh is used for testing the implicit EPSC UMAT implementation since it provides sufficient accuracy for this purpose.

**6.2.1 Effect of increment size on accuracy of the simulation results**

In order to determine an appropriate UMAT increment size the drawing simulation was first run with a $J_2$ material behavior i.e. the von Mises yield surface. The objective was to maximize the time increment, while preserving the accuracy of the simulation. The total equivalent strain at the material point was 0.48, split into 130 strain increments. The strain history in the form of three strain components has been extracted during the drawing step from the highlighted element in Fig 6b. Figure 7a shows the recorded strain history. The strain history is imposed along with zero stress 13, 23, and 33 components to generate the stress history by both explicit and implicit integration procedures. With sufficiently large number of increments in the explicit and implicit algorithms, both stress histories converge to the response with no appreciable difference as shown in Fig 7b and c. The difference is a bit lower if latent hardening and backstress are not considered (Fig. 7d). Here, the difference between stress histories calculated by the explicit and implicit algorithms is below 0.2%, as seen from Fig 7d. In these simulations, the number of steps in the integration procedure was set to 500 for the explicit procedure and to 100 for the implicit procedure for every increment coming from Abaqus. No sub-stepping was used for the integration at the single crystal level. The corresponding norm of imposed strain increment components is approximately $10^{-5}$ for the explicit and $5 \times 10^{-5}$ for the implicit procedure. They are intentionally set small for accuracy as these results are used as references for the increment size study presented below.
Apparently, the consideration of latent hardening and backstress in the model amplify the difference between the explicit and implicit EPSC. The difference starts to develop upon the strain path change. The introduction of the latent hardening values larger than the self-hardening into EPSC is coupled with numerical singularities [44, 54-56]. To overcome the numerical issues several procedures were developed in [39]. Close to singular matrices have large condition numbers and amplify differences in vector of knowns between the explicit and implicit EPSC models. The fitted backstress parameters from Table 2 produce a rapid increase of backstress, making the equations governing the evolution of backstress in rate form stiff. Even with very large number of steps overshoot can occur for some crystals. Disabling the backstress and latent hardening and comparing stress histories from the explicit and implicit EPSC models shows significantly lower mismatch (Fig 7d). The parameters for the dislocation based hardening law without latent hardening have been established in [39] and are reported in Table 3.

Table 3. Constitutive parameters for the evolution of slip resistance for \{111\}(1\{1\}) slip mode in AA6022-T4 without the consideration of latent hardening and slip system interaction in terms of evolution of dislocation densities.

<table>
<thead>
<tr>
<th>$L^{ss}$</th>
<th>$L^{ss'}$</th>
<th>$g^{ss}$</th>
<th>$g^{ss'}$</th>
<th>$\tau_0$[MPa]</th>
<th>$k_1[m^{-1}]$</th>
<th>$g$</th>
<th>$D[MPa]$</th>
<th>$q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>60</td>
<td>3.0 x10^8</td>
<td>0.1176</td>
<td>100</td>
<td>8</td>
</tr>
</tbody>
</table>

To study the sub-step sensitivity of the integration procedures, the number of sub-steps was varied and the results were compared against the “accurate” stress history generated with sufficiently large number of increments. In the explicit integration procedure the number of increments was decreased to 250, 100, 50 and 10 and the
obtained stress histories were compared against the stress history produced with 500 increments in Fig. 7e. Evidently, the explicit integration procedure quickly loses accuracy.

In the implicit integration procedure the number of sub-steps per imposed increment in strain from Abaqus was decreased to 10 and then to 2 and finally to 1, while no sub-stepping was used for the integration at the single crystal level. Next, the number of sub-steps in the integration of the single crystal response is varied for no sub-stepping per strain increment from Abaqus. The sub-increments were set to 100, 10, 2 and 1. The ability to perform the simulation with no sub-stepping involved at any level demonstrates that the overall implementation of FE-EPSC is numerically stable. The generated stress histories from these varying number of sub-steps were compared with the “accurate” stress history generated with 100 sub-steps in every imposed strain increment. The comparisons are presented in Fig. 7f, g and h. Evidently, the implicit code is less sensitive to the number of sub-steps than the explicit integration algorithm. For instance, same accuracy is achieved with implicit model having 2 sub-steps at either single crystal integration or in application of Abaqus strain increment as with explicit model with 100 steps in application of Abaqus increment.

The reduced number of steps in the implicit integration, compared to the explicit integration procedure, should be reflected in the computational time involved in simulations. The computational time comparison is shown in Fig 8a for different simulation cases already compared in terms of accuracy in Fig 7e, f and g. The plotted results are calculated as averages of three runs. The average error is calculated from
the difference between stress histories shown in Fig 7e, f and g. For instance, the average error for the explicit integration with 10 sub-steps is:

$$\text{Average error} \ [\%] = \frac{1}{ninc} \sum_{inc=1}^{ninc} \frac{2\|\sigma^{e,500}_inc - \sigma^{e,10}_inc\|}{\|\sigma^{e,500}_inc + \sigma^{e,10}_inc\|} \text{inc}$$  \hspace{1cm} (61)

where $ninc = 130$ is the total number of increments, $\sigma^{e,500}_inc$ is taken as the accurate reference stress at an increment $inc$ and $\sigma^{e,10}_inc$ is the calculated stress for the explicit integration with 10 sub-steps at the increment $inc$. The average error for the implicit code is calculated analogously. Increasing the number of sub-steps in the integration procedure results in the increase of the computational time and the decrease of the average error for both codes, as expected. For the implicit code, the accuracy of simulations saturates at 10 sub-steps (see the 1,10 implicit point in Fig 8a) in the single crystal integration, while applying the total strain increment from Abaqus in one step. Thus, further increase in the number of sub-steps in the single crystal integration scheme does not affect the accuracy, but significantly increases the computational time (see the 1,100 implicit point in Fig 8a). Also, increasing the number of sub-steps in the single crystal integration procedure is more computationally expensive than increasing the number of sub-steps for the Abaqus strain increment (compare the point 1,100 and 100,1 in Fig 8a). The comparison of computational times between the explicit and implicit code shows that for the same level of accuracy, the implicit code is faster. The ratio of the computational times between the explicit and implicit codes is plotted In Fig 8b. As is evident, the implicit code is at least 2 times faster than the explicit code for the same accuracy. The maximum gain in the computational efficiency is achieved with no
Fig. 7. (a) Imposed strain history. (b) The stress histories generated by the explicit and implicit integration algorithms with sufficient number of sub-steps and (c) the difference between them. (d) The difference like in (c) without considering the latent hardening and backstress effects. The effect of number of sub-increments on the accuracy of stress history in (e) explicit and (f and g) implicit integration algorithm. (h) The effect of the number of sub-increments in the implicit integration algorithm on stress history for the case without the backstress and latent hardening effects.
sub-stepping of an Abaqus strain increment and 2 sub-steps in the single crystal integration (see the point labeled as 1,2 in Fig 8b), giving the reduction of computational time by a factor of 8.6.

Fig. 8. (a) Computational time involved in the explicit and implicit integration procedures as a function of number of sub-steps. The number next to the explicit model points refers to the number of sub-steps in dividing the Abaqus strain increment, while the numbers next to the implicit model points refer to the number of sub-steps in dividing the Abaqus strain increment and the number of sub-steps used in the single crystal integration procedure, respectively. (b) Speed up of the implicit code relative to the explicit code for the same average error, calculated as the ratio of the explicit to the implicit computational times shown in (a).
As mentioned above, the objective in FE-EPSC simulations is to utilize increments driven by Abaqus meaning without introduction of any sub-stepping, although it is an option to specify in the model. The objective is also to use minimum number of sub-steps for the integration at the single crystal level, while retaining desired accuracy and reducing computational time required by explicit integration algorithm. In addition to user specified number of sub-steps in integration at single crystal level, intrinsic sub-incrementation due to activation of an additional slip system can occur. The results presented above show that the objectives of the developed implicit integration algorithm are well accomplished. For the cup drawing simulation we applied total increment from Abaqus and used 2 sub-steps in single crystal integration procedure.

6.2.2 Simulation results

The deformed mesh with contours of von Mises stress for the implicit EPSC UMAT is shown in Fig 9. Texture evolution introduces anisotropy in the mechanical response, which governs the shape evolution of the drawn cup (Fig 9a). After forming, the springback is simulated by fixing the node in the center of the formed cup and maintaining applied symmetries in the RD-ND and TD-ND planes. To suppress the occurrence of geometrical instabilities during springback step, artificial damping available in Abaqus is utilized [32] [41]. The resulting contours of von Mises residual stress are shown in Fig 9b. The shape of the cup after springback is compared with the shape of the cup after forming in terms of the nodal positions along RD direction and along the circumference of the cup edge in RD-TD plane in Fig 10a and b, respectively. In closing, it is worth mentioning that the overall computational time involved in the simulation using FE-EPSC was 34.2 hours. The job was run on a workstation with dual
socket Intel® Xeon® CPU E5-2695 v4 @2.1 GHz using 35 CPUs. The model is regarded as accurate but also as computationally intensive.

Fig. 9. Deformed mesh with contours of von Mises stress (a) after forming and (b) after springback. (c) Deformed mesh after springback.
Fig. 10. Prediction of shape: (a) the y-z profile of the drawn cup and (b) the circumference of the drown cup edge in x-z plane.

7. Conclusions

This work has developed an implicit integration algorithm for the EPSC polycrystal plasticity model. The rate forms of single crystal and polycrystal constitutive equations are replaced with corresponding incremental forms. An implicit integration algorithm at a single crystal level is used to derive the incremental form of the single crystal constitutive equation. In doing so, a system of non-linear equations is defined and conveniently solved using the fixed point method. With the developed solution procedure for single crystals, a suitable set of non-linear equations is derived from the self-consistent homogenization in incremental form and solved for single crystal strain increments using the Newton’s method. The implicit EPSC model is validated first using the original explicit EPSC model. Next, the implicit EPSC is implemented into a stress update algorithm within UMAT subroutine to facilitate the coupling with Abaqus. The implicit EPSC is capable of applying the total strain increment from Abaqus. Here, every
material point in the FE mesh is a polycrystal that deforms by anisotropic elasticity and crystallographic slip allowing for the heterogeneous deformation prediction that can occur across a sample as a result of work-piece geometry and material elastic and plastic anisotropy. The coupling is validated against the data from [44] for tension of single crystal Cu. Finally, a finite element simulation of cup drawing of AA6022-T4 with shell elements is performed to illustrate the potential and efficiency of the developed implicit multi-level framework. The evolution of texture, anisotropic hardening, BE, and nonlinear unloading were all taken into account in this simulation. The dimensional changes of the cup along with the non-uniform residual stress-strain distribution after drawing in the clamped condition as well as in the free state were predicted.

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Appendix A

In the notation used here, indices $s^+$ and $s^-$ refer to arbitrarily chosen positive and negative directions of slip systems, respectively. Both positive and negative directions are included in index $s$. The hardening law for the evolution of slip resistance is based on dislocation densities and is temperature and strain rate sensitive [57-62]. Here we summarize the formulation of dislocation based hardening law developed for prediction of anisotropy in mechanical response of aluminum alloy AA6022-T4 [39]. Reader is referred to [39] for detailed description of the hardening law.
The slip resistance is defined as:

$$\tau^s_c = \tau_0^s + \tau^s_{\text{forest}} + \tau^s_{\text{debris}}, \quad (A1)$$

where $\tau_0^s$ is an initial slip resistance, $\tau^s_{\text{forest}}$ is a contribution to slip resistance from statistically stored dislocations, $\tau^s_{\text{debris}}$ is a contribution to slip resistance from dislocations stored as debris. The forest contribution to slip resistance is:

$$\tau^s_{\text{forest}} = b^\alpha \chi \mu^\alpha \sqrt{\sum_{s't'} L_{s's'}^{s't'} \rho_{tot}^{s't'}} \quad (A2)$$

where $b^\alpha = 2.86 \times 10^{-10}$ m is the Burgers vector for aluminum, $\chi = 0.9$ is an interaction constant, $\rho_{tot}^{s'}$ is the total forest dislocation density for $s'$th slip system belonging to $\alpha$ slip mode ($s \in \alpha$) and $L_{s's'}^{s't'}$ is a strength interaction matrix [63, 64]. From single crystal experiments [48] the entries of strength interaction matrix have been evaluated to be 1 for coplanar slip systems and 1.4 for all other interactions. However, such strength interaction coefficients lead to the loss of ellipticity of the single crystal and macroscopic tangent modulus. A diagonalization procedure of hardening matrix is developed in [39] to treat the problem.

The debris contribution to slip resistance is:

$$\tau^s_{\text{debris}} = k_{\text{deb}} \mu^\alpha b^\alpha \sqrt{\rho_{\text{deb}}} \log \left( \frac{1}{b^\alpha \sqrt{\rho_{\text{deb}}}} \right) \quad (A3)$$

where $k_{\text{deb}} = 0.086$ is a material independent constant and $\rho_{\text{deb}}$ is the debris dislocation density [65].

The total dislocation density is:
\[ \rho_{\text{tot}}^s = \rho_{\text{for}}^s + \rho_{\text{rev}}^{s^+} + \rho_{\text{rev}}^{s^-}, \]  

(A4)

where \( \rho_{\text{for}}^s \) is the forward dislocation density and \( \rho_{\text{rev}}^{s^+} \) and \( \rho_{\text{rev}}^{s^-} \) are the reversible dislocation densities associated with the \( s^+ \) and \( s^- \) directions, respectively. Appropriate evolution laws are adopted for evolution of dislocation densities with shear strain and shearing direction [64, 66, 67]:

(If \( d\gamma^{s^+} > 0 \))

\[
\frac{\partial \rho_{\text{for}}^s}{\partial \gamma^s} = (1 - p) k_1^a \sqrt{\sum_{sr} g^{ssr} \rho_{\text{tot}}^{sr}} - k_2^a (\dot{\varepsilon}, T) \rho_{\text{for}}^s, \]  

(A5a)

\[
\frac{\partial \rho_{\text{rev}}^{s^+}}{\partial \gamma^s} = p k_1^a \sqrt{\sum_{sr} g^{ssr} \rho_{\text{tot}}^{sr}} - k_2^a (\dot{\varepsilon}, T) \rho_{\text{rev}}^{s^+}, \]  

(A6a)

\[
\frac{\partial \rho_{\text{rev}}^{s^-}}{\partial \gamma^s} = -k_1^a \sqrt{\sum_{sr} g^{ssr} \rho_{\text{tot}}^{sr}} \left( \frac{\rho_{\text{rev}}^{s^-}}{\rho_0^s} \right)^m, \]  

(A7a)

(If \( d\gamma^{s^-} > 0 \))

\[
\frac{\partial \rho_{\text{for}}^s}{\partial \gamma^s} = (1 - p) k_1^a \sqrt{\sum_{sr} g^{ssr} \rho_{\text{tot}}^{sr}} - k_2^a (\dot{\varepsilon}, T) \rho_{\text{for}}^s, \]  

(A5b)

\[
\frac{\partial \rho_{\text{rev}}^{s^+}}{\partial \gamma^s} = -k_1^a \sqrt{\sum_{sr} g^{ssr} \rho_{\text{tot}}^{sr}} \left( \frac{\rho_{\text{rev}}^{s^+}}{\rho_0^s} \right)^m, \]  

(A6b)

\[
\frac{\partial \rho_{\text{rev}}^{s^-}}{\partial \gamma^s} = p k_1^a \sqrt{\sum_{sr} g^{ssr} \rho_{\text{tot}}^{sr}} - k_2^a (\dot{\varepsilon}, T) \rho_{\text{rev}}^{s^-}, \]  

(A7b)

with the following initial conditions:

\[
\rho_{\text{for}}^s (\gamma^s = 0) = 10^{11} \text{ m}^{-2}, \quad \rho_{\text{rev}}^{s^+} (\gamma^s = 0) = 0 \quad \text{and} \quad \rho_{\text{rev}}^{s^-} (\gamma^s = 0) = 0, \]  

(A8)
where $k_1^\alpha$ is a coefficient controlling the rate of generation of statistically stored dislocations, $k_2^\alpha$ is a rate-sensitive coefficient for dynamic recovery [59], $p$ is a reversibility parameter having a value between 0 and 1, and $g^{ss'}$ is an interaction matrix, $m$ is a parameter accounting for the rate of dislocation recombination having value of 0.5 [68] and $\rho_0^s$ is the total dislocation density at the moment of shear reversal on the $s^{th}$ slip system [67]. Entries of the interaction matrix, $g^{ss'}$, describe the influence of dislocation density on the slip system $s'$ on the accumulation of forest dislocations on the slip system $s$ [64, 69, 70].

The rate-sensitive coefficient for dynamic recovery, $k_2^\alpha$, is:

$$\frac{k_2^\alpha}{k_1^\alpha} = \frac{\chi b^\alpha}{g^\alpha} \left( 1 - \frac{k_B T}{D^\alpha (b^\alpha)^3} \ln \left( \frac{k}{k_b} \right) \right),$$

(A9)

where, $k_B$ is the Boltzmann constant, $\dot{\epsilon}_0 = 10^7$ is a reference strain rate, $g^\alpha$ is an effective activation enthalpy and $D^\alpha$ is a drag stress. The debris dislocation density is evolved with:

$$\frac{\partial \rho_{deb}}{\partial \gamma^s} = q^\alpha b^\alpha \sqrt{\rho_{deb}} k_2^\alpha (\dot{\epsilon}, T) \rho_{tot}^s,$$

(A10)

where $q^\alpha$ is a dislocation recovery rate constant governing the amount of dislocations that get stored as debris, instead of being annihilated. Initial debris dislocation density is set to 0.1 $m^{-2}$.

In addition to dislocation-based evolution of slip resistance, a backstress on each slip system is introduced. The backstress was first implemented in EPSC in [29]. Here we use the same approach, while utilizing different backstress evolution laws. The
present backstress evolution laws and the backstress implementation in EPSC are discussed in detail in [39], while here we only provide a brief description.

The backstress is introduced to EPSC by altering the loading conditions (4a) and (4b):

\[
\sigma^c \cdot m^s - \tau_{bs}^s = \tau_c^s, \tag{A11}
\]

\[
\dot{\sigma}^c \cdot m^s - \dot{\tau}_{bs}^s = \dot{\tau}_c^s, \tag{A12}
\]

where \( \tau_{bs}^s \) is a backstress on a slip system. Analogues to Eq. (5), the backstress is assumed to evolve with shear rates:

\[
\dot{\tau}_{bs}^s = \sum_{s'} h_{bs}^{ss'} \dot{\gamma}_{s'}, \tag{A13}
\]

where \( h_{bs}^{ss'} \) is a backstress matrix. With introduction of the backstress the single crystal tangent stiffness retains the same form defined with Eq. (7), while the matrix \( X^{ss'} \), entering the tangent stiffness, becomes:

\[
X^{ss'} = h^{ss'} + h_{bs}^{ss'} + C^c \cdot m^s \otimes m^{s'}. \tag{A14}
\]

Before defining the backstress matrix, \( h_{bs}^{ss'} \), evolution laws for the backstress on a slip system, \( \tau_{bs}^s \), are introduced:

\[
\tau_{bs}^s = m^s \cdot \sigma_{bs}^c = \tau_{bs,sys}^s + 2 \sum_{s'} m^s \cdot m^{s'} \tau_{bs,sys'}^{s'}, \tag{A15}
\]

with

\[
\tau_{bs,sys'}^{s'} = \begin{cases} 
\tau_{bs,sys}^{s'} & \text{if } \tau_{bs,sys}^{s'} > 0 \\
0 & \text{if } \tau_{bs,sys}^{s'} < 0
\end{cases} \tag{A16}
\]
where $\sigma_{\text{bs}}^c$ is a backstress tensor formed by superimposing slip system sources of backstress, $\tau_{\text{bs,sys}}^{s'}$, and the sum over $s'$ spans over all slip systems and $s' \neq s$.

The slip system source of backstress is evolved with:

\[
(\text{if } d\gamma^s > 0 \text{ and } \tau_{\text{bs,sys}}^{s'} > 0)
\]

\[
\tau_{\text{bs,sys}}^{s'} = \tau_{\text{bs}}^{\text{sat}} \left(1 - \exp(-v\gamma^s)\right),
\]

\[
(\text{if } d\gamma^s > 0 \text{ and } \tau_{\text{bs,sys}}^{s'} < 0)
\]

\[
\tau_{\text{bs,sys}}^{s'} = -(A + 1)\tau_{\text{bs}}^{\text{sat}} \exp\left(-\frac{\gamma^s}{\gamma_b}\right) + \tau_{\text{bs}}^{\text{sat}}
\]

where $\tau_{\text{bs}}^{\text{sat}}$ is a saturation value for backstresses, $A$ is a parameter for asymmetric evolution of backstress on a slip system in two different directions $s^+$ and $s^-$, $\gamma_b$ and $v$ are material parameters. The shear strain $\gamma^s$ is recorded from the point of local load reversal.

Since the slip resistance and the backstress are defined as functions of shear strain, the hardening matrix, $h^{ss'}$, and the backstress matrix, $h_{\text{bs}}^{ss'}$, can be defined as:

\[
h^{ss'} = \frac{\partial \tau_{\text{bs}}^s}{\partial \gamma^{s'}}; \quad h_{\text{bs}}^{ss'} = \frac{\partial \tau_{\text{bs}}^{s'}}{\partial \gamma^{s'}}.
\]

The expressions for $h^{ss'}$ and $h_{\text{bs}}^{ss'}$ are provided in [39].
Introduction of realistic strength interaction coefficients, $L^{ss'}$, results in non-positive definiteness of hardening matrix, $h^{ss'}$ [39], meaning that the necessary condition for determination of shear rates on active slip systems is not fulfilled [56]. Therefore, issues in the solution procedure show up both at the single crystal and polycrystal level. To treat the major issue, which is loss of ellipticity of the polycrystal tangent stiffness, a diagonalization procedure is proposed in [39]. The procedure involves correction of hardening matrix, $h^{ss'}$, before evaluating the single crystal tangent stiffness with Eqs. (7) and (A14). It is assumed that the single crystal problem is solved, i.e. shear rates on active slip systems are known. The corrected hardening matrix, $h^{ss}_{d}$, is diagonal, ensuring positive definiteness:

$$h_{d}^{ss} = \frac{1}{\Delta \gamma_{s}} (\sum_{s'} h^{ss'} \Delta \gamma_{s'} - \sum_{s'} h^{ss'}_{off} \Delta \gamma_{s'}) \quad (A22)$$

where $h^{ss'}_{off}$ is a matrix formed from $h^{ss'}$ by setting the matrix entries along the diagonal to zero and $\Delta \gamma_{s'}$ are calculated increments in shear strain on active slip systems, while indices $s$ and $s'$ go over active slip systems.

References


durch oftmal wiederholte Beanspruchung, Mitteilungen aus dem mechanisch-technischen Laboratorium der k. polytechnischen Schule (1886) 1877-1836.


CHAPTER 3:

Modeling of sheet metal forming based on implicit embedding of the elasto-plastic self-consistent formulation in shell elements:

Application to cup drawing of AA6022-T4

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Modeling of sheet metal forming based on implicit embedding of the elasto-plastic self-consistent formulation in shell elements:

Application to cup drawing of AA6022-T4

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Abstract

This paper is concerned with multi-level simulations in sheet metal forming using a physically-based polycrystalline homogenization model that takes into account microstructure and the directionality of deformation mechanisms acting at single-crystal-level. The polycrystalline-level model is based on the elasto-plastic self-consistent (EPSC) homogenization of single-crystal behavior providing a constitutive response at each material point, within a boundary value problem solved using shell elements at the macro-level. A recently derived consistent tangent stiffness is adapted here to facilitate the coupling between EPSC and the implicit shell elements. The underlining EPSC model integrates a hardening law based on dislocation density, which is calibrated to predict anisotropic hardening, linear and non-linear unloading, and the Bauschinger effect upon the load reversal for AA6022-T4. To illustrate the potential of the coupled
multi-level FE-EPSC model, a simulation of cup drawing from an AA6022-T4 sheet is performed. Results and details of the approach are described in this paper.

*Keywords*: Sheet metal forming; Constitutive behavior; Anisotropic material; Shell elements; FE-EPSC
1. Introduction

In metal forming, metals are usually deformed to large plastic strains and develop non-uniform stress-strain fields [1-5]. It is well known that the glide of dislocations (crystallographic slip) accommodates most of the plastic strains. Crystallographic slip induces anisotropy in the mechanical response by evolution of texture and dislocation structure. Additionally, intra- and inter-granular elastic deformation fields develop playing an important role in the overall deformation process and, in particular, during unloading and strain path changes [6-8]. For example, upon application of strain in the reversed direction, the material exhibits non-linear unloading first [2] and then a reduction in yield stress from that reached at the end of pre-straining known as the Bauschinger effect (BE) [6]. The hardening rate that follows with continuation of straining in the reverse direction is usually lower from that during pre-straining. This stress offset between forward and reversed flow is referred to as the permanent softening [9, 10]. These characteristics of material behavior are governed by the evolution of the underlying physical phenomena created by crystallographic slip within the material microstructure.

The nonlinear unloading is facilitated by partial re-emission of dislocations impeded by grain boundaries during forward loading [11]. The impeded dislocations are referred to as the dislocation pile-ups. The dislocation re-emission from the pile-ups is facilitated by the relaxation of micro backstresses acting in vicinity of pile-ups. The higher the pre-strain level the higher deviation from the linear elastic unloading behavior. Hence, to predict the non-linear unloading, a constitutive law in use must accurately model pre-straining. The BE has been extensively studied in both single
crystal [12] and polycrystalline metals [13, 14]. The origin of BE is established to be backstress. The built up backstress acts against the applied stress during forward loading. Upon loading in the reverse direction, the applied stresses combine with the backstresses, which results in a drop of the reverse yield stress. The change in the hardening rate after load reversal originates from the annihilation/dissolution of dislocations formed during the primary deformation path [13, 15].

We have recently showed that a hardening law explicitly based on dislocation density evolution and slip system backstress evolution implemented within the elasto-plastic self-consistent (EPSC) homogenization scheme performs well in capturing the above described phenomena [16-18]. In turn, this provided an incentive for incorporating the EPSC-based user material (UMAT) subroutine into a finite element (FE) framework (Abaqus) to facilitate process design and mechanical evaluation of components. Several crystal plasticity models have been used within FE codes to simulate bulk forming operations [19-24]. The strategy of embedding the EPSC model at the meso-scale level in an implicit FE analysis was described in [25]. The overall model was termed FE-EPSC and its capabilities demonstrated on a few case studies in bulk metal forming. In an implicit nonlinear FE formulation, the material constitutive model provides the stress and tangent stiffness matrix. The tangent stiffness matrix (Jacobian) in E-EPSC was obtained analytically facilitating fast convergence towards stress equilibrium.

In this paper, we combine these recent advances and present the first successful implementation of the EPSC polycrystalline model within implicit shell finite elements. Sheet metal forming simulations are typically performed using shell elements because
of their computational efficiency, which was the main motivation to enable the FE-EPSC model to provide the constitutive response for shell elements. To illustrate the potential of the coupled multi-level FE-EPSC model, a simulation of cup drawing from an AA6022-T4 sheet is carried out. The simulation subjects the sheet metal to be under a multi-axial deformation path during the drawing step and the subsequent springback unloading step representing a stringent test for the model.

2. Material

The material used in the present work is AA6022, which is a heat treatable low copper, Al-Si-Mg alloy from Alcoa. The material was in the temper T4 condition. Figure 1a depicts pole figures of initial texture in the sheet [16]. The presence of a cube texture component is evident from the pole figures. The average grain size in the material was approximately 50 μm. The alloy was tested under cycle tension-compression to several strain levels as shown in Fig. 1b.

The standalone EPSC model was initialized with the measured texture and adjusted to reproduce the experimentally measured stress-strain curves in earlier work [16, 25]. Figure 1b shows that the model successfully captures the anisotropic hardening during primary loading, BE, nonlinear unloading, and hardening in the reverse direction. Model description along with the material parameters can be found in [16, 25]. Here, we present the EPSC model for deformation of polycrystalline metals implemented as a UMAT subroutine in Abaqus, providing the necessary constitutive relationship between stress-strain for shell elements. Each integration point of the shell element model is considered as a polycrystalline material point with a given initial
texture represented using 100 weighted orientations that evolve with deformation. The implementation is described in the next section.

**Fig. 1.** (a) Pole figures showing initial texture in AA6022-T4. (b) Cyclic tension-compression stress-strain response of AA6022-T4 to 2%, 5% and 10% of tensile engineering pre-strain. Comparison of the EPSC model predictions (dashed line) and measurements (solid line) is shown.

3. **Formulation of the FE-EPSC UMAT for shell elements**

The EPSC material model is based on the Eshelby’s equivalent inclusion method. Each grain is treated as an inhomogeneity embedded in a homogenous effective medium (HEM), which is representative of the polycrystalline behavior. Therefore, stress and strain fields inside each grain are uniform and are calculated by considering interaction between the inhomogeneity (grain) and the HEM. The compatibility and equilibrium are satisfied in an average sense, meaning that the mean of stress and strain over all grains is equal to the stress and strain of the HEM.
The formulation of shell elements implies state of plane stress at each point of an FE model. Three strain components based on a displacement increment of an FE model are provided as input to the FE-EPSC UMAT subroutine. The UMAT subroutine provides the three stress components, the Jacobian matrix, and updated state variables at the end of a given strain increment. In the shell element formulation in Abaqus, tensors are expressed in the local frame of elements, which implies that the macroscopically applied spin at each integration point is zero. As mentioned above, the FE-EPSC UMAT developed previously for general three dimensional (3D) stress state [25] is adopted here to work with shell elements, which assume the state of plane stress.

The following constitutive relation in its rate form is integrated within UMAT:

\[
\dot{\sigma} = L \dot{\varepsilon} + \frac{1}{N} \sum_{i=1}^{N} (\omega_i \dot{\sigma}_i + \delta \sigma_i \Gamma_i), \tag{1}
\]

where \( L \) is the elasto-plastic instantaneous stiffness of a polycrystal consisting of single crystals \( c \), \( \sigma^c \) is the Cauchy stress per crystal \( c \), \( \dot{\varepsilon} \) is the total strain rate, \( \dot{\sigma} \) is the macroscopic Cauchy stress rate, and \( \omega^c \) is the lattice spin rate of a crystal \( c \). The lattice spin rate of a grain is defined as: \( \omega^c = \omega^{app} + \Pi^c - \omega^{p,c} \), where \( \omega^{app} \) is the macroscopically applied spin, \( \Pi^c \) is the rigid body spin coming from the antisymmetric part of the Eshelby tensor, and \( \omega^{p,c} \) is the plastic spin due to crystallographic slip. Note that with \( \omega^{app} = 0 \), the lattice spin is not zero, and thus, texture evolves with deformation. The equation is integrated numerically from \( t \) to \( t + \Delta t \) and the following expression for stress at the end of the time increment is derived:

\[
\sigma_{t+\Delta t} = \sigma_t + \frac{\Delta t}{N} \sum_{i=1}^{N} L_i \dot{\varepsilon}_i + \frac{\delta}{N} \sum_{i=1}^{N} (\omega^c_i \Delta t \sigma^c_i + (< \omega^c_i \Delta t \sigma^c_i > + (< \omega^c_i \Delta t \sigma^c_i > T)), \tag{2}
\]
where N is the number of sub-increments in UMAT within a given time increment from Abaqus. Tensor equations (1) and (2) represent a system of six independent scalar equations. For the shell element formulation, the system of six equations reduces to a system of three equations for the evaluation of three components of stress tensor, which are required by Abaqus:

\[
\begin{bmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{12}
\end{bmatrix}_{t+\Delta t} = \begin{bmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{12}
\end{bmatrix}_t + \frac{\Delta t}{N} \sum_{i=1}^{N} \begin{bmatrix}
L_{11} & L_{12} & L_{13} & L_{14} & L_{15} & L_{16} \\
L_{21} & L_{22} & L_{23} & L_{24} & L_{25} & L_{26} \\
L_{61} & L_{62} & L_{63} & L_{64} & L_{65} & L_{66}
\end{bmatrix}_i \begin{bmatrix}
\dot{\epsilon}_{11} \\
\dot{\epsilon}_{22} \\
\dot{\epsilon}_{33} \\
\dot{\epsilon}_{12} \\
\dot{\epsilon}_{23} \\
\dot{\epsilon}_{13}
\end{bmatrix}_i
\]

\[
\frac{1}{N} \sum_{i=1}^{N} \begin{bmatrix}
T_{11} \\
T_{22} \\
T_{12}
\end{bmatrix}_i ،
\]

where \( T_{11} \), \( T_{22} \) and \( T_{12} \) are components of a symmetric 2\(^{nd}\) rank tensor \( T \), which is:

\[
T = < W_i^c \Delta t \sigma_i^c > + < (W_i^c \Delta t \sigma_i^c)^T > .
\]

Although at the homogenized polycrystal level there is a plane state of stress, each constituent crystal is under a full 3D stress state. Note that there are three independent strain rate components at macroscopic level. These are \( \dot{\epsilon}_{11}^i, \dot{\epsilon}_{22}^i \) and \( \dot{\epsilon}_{12}^i \). The remaining strain rate components \( \dot{\epsilon}_{33}^i, \dot{\epsilon}_{23}^i \) and \( \dot{\epsilon}_{13}^i \) can be expressed in terms of the former three strain rate components using the three equations for zero stress from Eq. (2) at an instant \( i \). After several simple algebraic manipulations we arrive to the expression:

\[
\Delta t \begin{bmatrix}
\dot{\epsilon}_{33} \\
2\dot{\epsilon}_{23} \\
2\dot{\epsilon}_{13}
\end{bmatrix}_i = - \begin{bmatrix}
L_{33} & L_{34} & L_{35} \\
L_{43} & L_{44} & L_{45} \\
L_{53} & L_{54} & L_{55}
\end{bmatrix}_i^{-1} \left( \begin{bmatrix}
L_{31} & L_{32} & L_{36} \\
L_{41} & L_{42} & L_{46} \\
L_{51} & L_{52} & L_{56}
\end{bmatrix}_i \begin{bmatrix}
\Delta \epsilon_{11} \\
\Delta \epsilon_{22} \\
2 \Delta \epsilon_{12}
\end{bmatrix}_i + \begin{bmatrix}
T_{33} \\
T_{23} \\
T_{13}
\end{bmatrix}_i \right).
\]
Taking into account Eq. (5), the final expression for the three stress components in terms of the independent macroscopic strain is:

\[
\begin{bmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{12}
\end{bmatrix}_{t+\Delta t} = \\
\begin{bmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{12}
\end{bmatrix}_t + \\
\frac{1}{N} \sum_{i=1}^{N} \left( \begin{bmatrix}
L_{11} & L_{12} & L_{16} \\
L_{21} & L_{22} & L_{26} \\
L_{61} & L_{62} & L_{66}
\end{bmatrix} \begin{bmatrix}
\Delta \varepsilon_{11} \\
\Delta \varepsilon_{22} \\
2 \Delta \varepsilon_{12}
\end{bmatrix} - \\
\begin{bmatrix}
L_{13} & L_{14} & L_{15} \\
L_{23} & L_{24} & L_{25} \\
L_{63} & L_{64} & L_{65}
\end{bmatrix}_i \left( \begin{bmatrix}
L_{13} & L_{14} & L_{16} & L_{23} & L_{24} & L_{26} & L_{63} & L_{64} & L_{66}
\end{bmatrix}_i \begin{bmatrix}
\Delta \varepsilon_{11} \\
\Delta \varepsilon_{22} \\
2 \Delta \varepsilon_{12}
\end{bmatrix} + \begin{bmatrix}
T_{33} \\
T_{23} \\
T_{13}_i
\end{bmatrix}_i \right) \right) + \\
\frac{1}{N} \sum_{i=1}^{N} \begin{bmatrix}
T_{11} \\
T_{22} \\
T_{12}_i
\end{bmatrix}_i
\]  

(6)

The strain increment \((\Delta \varepsilon_{11} = \Delta \varepsilon_{11}^{Abaqus}, \Delta \varepsilon_{22} = \Delta \varepsilon_{22}^{Abaqus}, \text{and } 2\Delta \varepsilon_{12} = \Delta \varepsilon_{12}^{Abaqus})\) is provided by Abaqus based on the boundary conditions imposed on an FE model representing sheet forming. To this end, the EPSC model is interrogated using the mixed boundary condition consisting of \(\sigma_{33} = 0, \sigma_{13} = 0, \sigma_{23} = 0, \Delta \varepsilon_{11}, \Delta \varepsilon_{22}, \text{and } \Delta \varepsilon_{12}\) at each trial strain increment.

A detailed derivation of the consistent tangent modulus for 3D stress state is given in [25]. In addition to the reduction from 3D stress state for the continuum element formulation to two dimensional (2D) stress state for the shell element formulation, the latter formulation discards the dependence of \(T\) on the strain increment due to the fact that there is no macroscopically applied spin. As a result, the Jacobian matrix is:
\[ J = \frac{\partial \Delta \sigma}{\partial \Delta \epsilon} = \]
\[
\frac{1}{N} \sum_{i=1}^{N} \left( \begin{bmatrix}
L_{11} & L_{12} & L_{16} \\
L_{21} & L_{22} & L_{26} \\
L_{61} & L_{62} & L_{66}
\end{bmatrix}_i - \begin{bmatrix}
L_{13} & L_{14} & L_{15} \\
L_{23} & L_{24} & L_{25} \\
L_{63} & L_{64} & L_{65}
\end{bmatrix}_i \right) \begin{bmatrix}
L_{33} & L_{34} & L_{35} \\
L_{43} & L_{44} & L_{45} \\
L_{53} & L_{54} & L_{55}
\end{bmatrix}_i^{-1} \begin{bmatrix}
L_{31} & L_{32} & L_{36} \\
L_{41} & L_{42} & L_{46} \\
L_{51} & L_{52} & L_{56}
\end{bmatrix}_i. \quad (7)
\]

4. Results and discussion

We present a cup drawing simulation from an AA6022-T4 sheet as an application case study to demonstrate capabilities of the shell element FE-EPSC UMAT formulation. Schematic showing the geometry of the simulation setup is shown in Fig. 2a. The simulation consists of four steps: (1) establishing the contact, (2) applying the blank holding force of 2.5 kN, (3) forming the cup by displacing the punch to a stroke of 12 mm, and (4) springback, which is simulated by removing the contact between blank and other parts. The loading is axisymmetric. However, due to the presence of orthotropic sample symmetry in texture (see Fig. 1a) one quarter of the blank was modeled with the appropriate symmetry boundary conditions. Figure 2b shows the FE quarter model of the initial blank consisting of 1225 S4R and 25 S3R shell elements. The S3R elements are triangular shell elements used at the center of the blank. The die, punch, and blank holder were modeled as analytical rigid surfaces. The coefficient of friction was taken to be 0.1. As mentioned earlier, the stand-alone EPSC model was calibrated for AA6022-T4 data in [16, 25] and is used here. The predicted results of the model are described next. Figure 3 shows contours of predicted von Mises stress after drawing. Due to the presence of the cube texture component where the crystallographically soft <001> direction is aligned with the sample axis of the sheet (Fig. 1a), the response is softer in RD and TD then at any other direction in between the RD and TD. The contours show that the response is the hardest at 45°. Evidently, the
model is capable of capturing the texture induced anisotropy in the mechanical response of the AA6022-T4 sheet.

Fig. 2. Simulation setup: (a) deep drawing geometry and (b) FE quarter model of the initial blank containing 1250 shell element. 50 elements are along the diameter and 25 elements are along the circumference of the blank.

Fig. 3. Contours of von Mises stress at the end of forming.

Next, we perform the springback unloading simulation of the drawn cup. The free state of the drawn cup is imposed by fixing one node in the center of drawn cup. The
Springback simulation was numerically more challenging to perform due to an instability that showed up during the springback step. The instability is localized and is of geometrical nature. By definition, an instability is the phenomenon in which a small increase in load causes a disproportionately large increase in deformation. We were able to stabilize the springback simulation by the artificial damping procedure offered by Abaqus for such numerical problems [26]. The procedure involved applying a viscous force, $f_v$, at each node. The global vector of viscous forces per node $n$ is calculated using the following product: $f_v^n = cM^*v^n$, where $v^n$ is a global vector constructed from nodal velocities $v^n = \frac{\Delta u^n}{\Delta t}$, $c = 0.02$ is a damping factor, and $M^*$ is an artificial mass matrix of unit density. The mass matrix is assembled from lumped element mass matrices. The lumped mass matrix is obtained by adding each row of the consistent mass matrix: $M^e = \int V e N^T N dV$, on to the diagonal, where $N$ is the element shape function matrix. The use of mass matrix is analogous to dynamic analysis where the inertial forces are obtained by multiplication of the mass matrix with vectors of nodal acceleration. The use of constant value of damping factor is the preferred way of suppressing the local instability because other stabilization methods offered by Abaqus often fail or produce inaccurate results [27]. The viscous force takes the direction of velocity at each node and is applied as negative of it to the nodal force balance (i.e. in the direction of externally applied nodal forces).

The maximum value of viscous force in the model is compared to the average value of forces present at nodes and the energy dissipated through viscous damping is compared to the total strain energy measured with respect to the state at the end of forming to check whether the viscous force artificially affects the results in an
appreciable manner. The change in energy dissipated through stabilization during springback can be calculated using $\Delta E_{st} = \int_{t_{start}}^{t_{end}} \mathbf{f}_v \cdot \mathbf{v}^n dV dt$ while the change (release) in the total strain energy during springback is simply $\Delta E_t = \int_{t_{start}}^{t_{end}} \sigma \cdot \varepsilon dV dt$. The viscous forces are below 0.254% of the average force and the energy dissipated through stabilization is below 0.756% of total strain energy change during springback. According to the Abaqus manual, the maximum value allowed for the energy dissipated through stabilization is 5%. The viscous forces are at maximum with respect to average nodal forces at the end of the springback simulation step. Although the effect of stabilization appears to be minimal, an additional step is performed with very low damping factor of $c = 0.00002$ in order to relieve the residual viscous forces. Figure 4 shows the simulation results. Contours of von Mises residual stress at the end of springback and after relieving residual viscous forces are shown. It can be seen that the artificially added force does not appreciably influence the results while facilitating the completion of the springback unloading simulation step. Dimensional changes are depicted in Fig. 5. It can be seen that the cup deflects during the springback and that the damping procedure does not appreciably influence the predictions. The account of anisotropic elastic strains by the model as part of the deformation of individual crystals was the key for the prediction of the free state springback deflection.

Pole figures showing predicted textures at several spatial locations (bottom, wall, and flange) along the three directions (RD, TD, and at 45°) after forming of the cup are presented in Fig. 6. The results suggest that texture evolves slightly more in the wall region than at bottom and in the flange region for the RD and TD directions, while the trend is opposite for the 45° direction.
In closing, it is worth mentioning that the overall computational time involved in the simulation using FE-EPSC was 34 hours. The job was run on a workstation Intel® Xeon® CPU X5650 @2.67 GHz using 10 CPUs. The model is regarded as accurate but also as computationally intensive.

Fig. 4. Contours of von Mises stress after (a) the springback simulation and (b) relieving the residual viscous forces artificially added to stabilize the springback simulation.

Fig. 5. Prediction of shape change after springback: (a) the y-z profile of the drawn cup and (b) the circumference of the drawn cup flange.
Fig. 6. (a) Initial texture represented using 100 weighted orientations, which were embedded at each FE integration point. (b) Predicted textures after forming at selected spatial locations in the center along the thickness direction of the cup. (c) Deformed mesh showing the spatial locations of recorded textures.
5. Conclusions

In this work, we have presented a numerical implementation of the EPSC crystal plasticity model in shell finite element framework. To this end, we have adapted the recently developed 3D FE-EPSC model to a plane stress implementation as required by shell elements. Every material point in the FE shell mesh is a polycrystal that deforms by anisotropic elasticity and crystallographic slip allowing for the heterogeneous deformation prediction that can occur across a sample as a result of work-piece geometry and material elastic and plastic anisotropy. The evolution of texture, anisotropic hardening, BE, and nonlinear unloading were all taken into account by the model. The model is applied to a case study of cup drawing in the sheet metal forming of AA6022-T4. The multi-level model was capable of performing drawing and the subsequent springback unloading. However, the stabilization procedure was found necessary to facilitate the unloading step. It was quantified that the procedure did not appreciably influence the results. The dimensional changes of the cup along with the non-uniform residual stress-strain distribution and texture after drawing in the clamped condition as well as in the free state were predicted.

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CHAPTER 4:

A dislocation density based elasto-plastic self-consistent model for the prediction of cyclic deformation: Application to AA6022-T4

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A dislocation density based elasto-plastic self-consistent model for the prediction of cyclic deformation: Application to AA6022-T4

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Abstract

We develop a polycrystal plasticity constitutive law based on the elasto-plastic self-consistent (EPSC) theory for the prediction of cyclic tension-compression deformation. The crystallography based model integrates a dislocation based hardening model and accounts for inter-granular stresses and slip system level backstresses, which make it capable of capturing non-linear unloading and the Bauschinger effect (BE). Furthermore, the model features dissolution of dislocation population upon the load reversal, which enables it to predict the change in hardening rate during reverse loading from that during forward loading. To demonstrate these capabilities of the model, we investigate elasto–plastic behavior of AA6022-T4 sheets under in-plane cyclic tension–compression. From a set of carefully performed cyclic tests to several strain levels, we observe that the material exhibits (1) a typical decreasing hardening rate during forward loading, (2) a linear followed by non-linear unloading upon the load
reversal, (3) a transient softening followed by rapid work hardening (the BE), and (4) a decrease in subsequent hardening rate during reverse loading (the permanent softening phenomenon). To predict these effects, we calibrate the model to establish a set of material parameters using a portion of the measured data. The remaining measured data is used for verification of the model. We show that using the single set of material parameters, the developed model is capable of predicting all the particularities pertaining to the cyclic deformation of the material with great accuracy. From the favorable comparison of the predictions and experimental data, we infer first that the non-linearity of unloading increases with the amount of pre-strain, next that the backstresses have a dominant effect in capturing non-linear unloading while both the backstresses and inter-granular stresses govern the BE, and finally that the inclusion of reversible dislocation motion is the key for capturing hardening rates during reverse loading.

*Keywords*: B. Bauschinger effect; B. Residual stress; B. Backstress; A. Dislocations; B. Crystal plasticity
1. Introduction

Numerical simulations play a major role in optimization of metal forming processes and evaluation of component performances in service. Accuracy of such simulations is highly dependent on the accuracy of a material model, which is integral in such numerical tools. Since metal forming processes involve non-monotonic and multi-axial deformation paths, it is necessary for the material model to be sensitive to such deformation path changes. For example, the springback behavior of forming parts after removal from a die depends on the elasto-plastic behavior of the material during unloading [1, 2]. The bending-unbending behavior of sheets drawn over a die radius depends on the elasto-plastic behavior of the material during tension followed by compression [2, 3].

In addition to the flow stress and concomitant work hardening rate during forward monotonic loading, material models sensitive to strain reversals must capture the following directional effects: (1) linear and non-linear unloading, (2) transient in yield stress and work hardening rate immediately after re-yielding known as the Bauschinger effect (BE), and (3) subsequent work hardening rate, which is usually different from that during the forward loading. These effects are attributed to the evolution of the underlying physical phenomena and the microstructure, which are briefly summarized below.

Non-linear unloading behavior refers to a small departure from a linear elastic material law during unloading [2, 4]. The total unloading strain comprises an initial elastic component followed by small scale re-yielding attributed to a dislocation relaxation phenomenon [4-8]. This small scale back flow during unloading is a
consequence of the presence of micro backstresses formed during forward loading. These micro backstresses arise from dislocation pile-ups, which consist of dislocations incorporated into grain boundaries during forward loading. Upon unloading, the micro backstresses relax, giving rise to a micro plastic strain in the reverse direction. This micro plastic strain is accommodated by a partial re-emission of the dislocations from the grain boundary pile-ups [6, 8]. Level of plastic deformation before unloading is expected to influence the magnitude of deviation from the linear unloading behavior. Therefore, capturing the effect of non-linear unloading by constitutive models requires modeling of prior plastic deformation.

The BE [9] refers to the change in yield strength followed by rapid hardening of a material deformed in tension (compression) and subsequently in compression (tension). The BE effect has been observed in the deformation of polycrystals [10-12] as well as single crystals [13-16] and its phenomenology and microstructural descriptions are well documented [17, 18]. Similar to non-linear unloading, it arises from the local deviation from an applied stress due to backstresses having inter- and intra-granular sources. The intra-granular backstress sources explain the BE in single crystals. In contrast to non-linear unloading of polycrystals, dislocation grain boundary pile-ups cannot be the origin of these backstresses in single crystals. Incompatibility between hard dislocation walls of high dislocation density separated by soft regions of low dislocation density develops long-range internal stresses (LRIS) (aka intra-granular stresses or type III stresses) [19, 20]. During forward deformation LRIS are induced in the opposite direction from that of the applied stress. Upon reloading, LRIS combine with the reversed loading stress, causing a drop in the onset of plastic deformation. Orowan's
theory, which states that there is an anisotropy in resistance to dislocation motion between forward and reverse motion, offers an additional explanation of the BE in single crystals. Dislocations move easier in the reversed direction because obstacles on the same path have been overcome during the forward motion [21]. The BE effect in polycrystals is caused by that in single crystals, by the existence of additional sources of backstresses, and by inter-granular stresses (type II stresses). The additional sources of backstresses are the pile-ups at grain boundaries [22, 23] and any non-deforming particles [24, 25]. Depending on the crystallographic orientation with respect to the loading axis, the yield strengths of different grains are divergent with some grains being harder and some being softer. The inter-granular stresses build up due to strain incompatibility between adjacent hard/soft grains of different crystal orientations during forward loading. Similarly these stresses assist the stress applied in the reverse direction, which is reflected in the drop of the yield stress [22, 26]. Therefore, both intra- and inter-granular stresses give rise to the BE in polycrystals. These stresses are strongly linked to the concurrent evolutions of crystallographic and morphological texture with plastic strain, which induce the plastic anisotropy.

Following the BE, a change of the work hardening rate occurs during reverse loading to large strains [10, 27-29]. This change manifests in an offset between the forward and the reverse flow stresses [21, 30, 31] and is referred to as permanent softening. The effect originates from the annihilation/dissolution of loosely tangled dislocation contained in dislocation substructures formed during the primary deformation path, as well as slow buildup of new dislocation substructures during deformation in the opposite direction.
Incorporation of the above summarized effects in constitutive models represents a challenging task. Clearly, simple phenomenological material models based on isotropic continuum plasticity are insufficient [32]. A range of more sophisticated phenomenological models have been developed to quantitatively predict the BE through a combination of isotropic and linear or non-linear kinematic hardening laws [33-38]. These phenomenological models, while computationally efficient and relatively easy to implement within commercial finite element codes, are not physically based and therefore do not directly account for the mechanistic sources of backstresses, or even distinguish between inter- and intra-granular contributions. A significant limitation of these models is that it is difficult to find the values of the material parameters, demanding expensive and complex mechanical tests and inverse methodologies to find the parameters [39]. Additionally, these models apply to a specific initial material state and to the specific loading conditions used in the model fitting process.

An attractive alternative is the physics-based crystal plasticity theory, which is based on the crystallography of various deformation mechanisms and considers crystallographic texture as an input state variable that evolves with plastic strain. Such physical description of plastic deformation naturally incorporates development of the plastic anisotropy caused by textural and microstructural changes during deformation [40]. Polycrystal plasticity models link response of constituent single crystals to the response of a polycrystalline aggregate. For this purpose different homogenization schemes exist ranging from an upper-bound Taylor [41-51], to lower-bound Sachs [52-54], to mean-filed self-consistent [55], and finally to full-field finite element models [56-60]. To facilitate simulations under heterogeneous plastic strains, these polycrystal
codes are further coupled with commercial finite element codes to operate at a FE integration point [61-67]. Polycrystal plasticity models intrinsically account for anisotropic elasto-plastic behavior of the material and, depending on the selected homogenizations, are capable of calculating the inter-granular sources of backstress. While the Taylor homogenization predicts large inter-granular stresses, the Sachs model develops no such stresses. Though finite element homogenization would lead to the most accurate estimates of backstresses, it is computationally impractical. Self-consistent homogenization provides the best compromise between computational speed and accuracy. In addition to predictions of mechanical response, the added benefits of polycrystal plasticity models include their ability to provide valuable information about texture evolution as well as physical insights into active deformation modes. Moreover, these models are not constrained to an initial material state or to a specific deformation path, and therefore are much more predictive and robust than macroscopic plasticity models.

The elasto-plastic self-consistent (EPSC) model [68] is among the most widely applied crystal plasticity models for the prediction of inter-granular stresses. However, the inherent inter-granular stresses predicted by EPSC were found insufficient to capture subtleties of cyclic deformation of stainless steel [69]. The primary reason for the poor predictions is lack of backstress kinematic hardening effects. More recently, backstresses at the slip system level have been incorporated within the Voce hardening law in EPSC, resulting in successful predictions of small strain cyclic deformation [70]. Since this model was implemented within the phenomenological Voce hardening law, it
has been unable to capture subsequent hardening behavior during reloading to large strains as a function of the level of pre-loading strain.

On the other hand, the visco-plastic self-consistent (VPSC) model [55] was used with an extended Voce hardening law for modeling the BE [71] and with a dislocation based hardening law for modeling both the BE and subsequent work hardening rates to large strains upon strain reversal [28, 72, 73]. The key feature of the later model is that it includes a reversible dislocation population that annihilates upon strain reversal, enabling reverse hardening rate predictions. The backstresses in VPSC cannot be entirely related to physical phenomena, since VPSC neglects effect of inter-granular stresses. Moreover, due to the absence of elasticity VPSC cannot model the unloading effects.

Taking advantages of the above developments in EPSC and VPSC, we present a comprehensive dislocation based hardening law in EPSC for cyclic deformation. The law is directional at the slip system level and evolves the slip resistance and internal stresses with microstructure rearrangements upon load reversal. Specifically, it accounts for the inter-granular stresses and the backstress kinematic hardening at the slip system level for the predictions of non-linear unloading and the subsequent BE upon reloading. The model considers dislocation dissolution for the prediction of hardening rates during loading in the reverse direction. To demonstrate predictive capabilities of the model, we characterize the cyclic tension-compression response of the AA6022-T4 alloy and use the dataset for calibration and verification. We show that the new hardening law within the EPSC polycrystal model is capable of capturing all the particularities associated with the cyclic response of the material. Since the
microstructural features are incorporated in the hardening law, the model successfully predicts the cyclic material behavior as a function of loading directions and level of pre-strain. We found that the non-linearity of unloading increases with the amount of pre-strain; the backstresses control the non-linear unloading while both the backstresses and inter-granular stresses govern the BE; and that the reversible dislocation motion plays the major role in hardening during reverse loading.

The paper is organized as follows. Cyclic tension-compression measured data and characterization data of the initial microstructure of AA6022-T4 are presented in section 2. The new EPSC model is described in section 3. Results of the cyclic simulations and role of the individual effects through the comparisons between simulated and measured cyclic curves are presented in section 4. Conclusions are presented in section 5.

2. Material characterization and cyclic tension-compression measurements

The material investigated here is a sheet of 6022 heat treatable low copper, Al-Si-Mg alloy [74, 75]. This widely used alloy offers an excellent combination of strength and formability. The material was in the temper T4 condition (AA6022-T4). Figure 1a shows an orientation map collected using the electron backscattered diffraction (EBSD) orientation imaging method to depict the grain structure of the alloy. The average grain size in the material is approximately 50 µm with grains slightly elongated in the rolling direction (RD). To acquire information about the initial crystallographic texture in the material, multiple EBSD scans were collected over an area of several square millimeters. Figure 1b shows the corresponding pole figures. Presence of a strong cube texture component is evident from the pole figures.
Fig. 1. (a) Orientation map and (b) pole figures of the initial microstructure and texture of the AA6022-T4 sheet.

The focus of the present paper is to develop a constitutive law sensitive to strain reversals. Various experimental methods have been developed to test materials under such conditions including forward and reverse torsion [10, 76], forward and reverse simple shear [77], tension followed by torsion [78], tension followed by simple shear [79, 80], and tension followed by compression [1, 4, 81-83]. Here, the AA6022-T4 alloy was tested under the cycle tension-compression to several strain levels.

Specimens were cut out of sheets of AA6022-T4 with orientations along the rolling direction (RD) and along the transverse direction (TD). For cyclic tension-compression, the specimens were 130 mm long and 12.5 mm wide with a 12.5 mm
gauge length by 10 mm in width. To make sure that the tension portion of the cyclic tension-compression curves matches regular tension test data, additional tensile specimens were made and tested. Both the cyclic tension-compression and tension tests were performed on the MTS machine 858 Table Top System. A set of specialized fixtures were used for the cyclic tests as described in [81, 82]. Cyclic tests at strain rate of 0.004 s$^{-1}$ were performed to 2% strain for the RD and TD samples and to 5% and 10% for the RD samples.

Figure 2 depicts several representations of the measured true stress–true strain curves including the normalized strain hardening rate plots. It is observed that the alloy exhibits a classical decreasing hardening rate throughout the response in tension, which is typical for materials in which the plastic deformation is accommodated by crystallographic slip. Upon unloading, the material exhibits an initial linear portion and a subsequent non-linear portion of unloading behavior (Fig. 2a and b). The non-linear portion of the unloading curve is a function of plastic strain, and it increases with strain (Fig. 2a). Figure 2c, d and e depict the hardening behavior. The overall decrease of the hardening rate during the reverse loading in compression is more pronounced than forward loading and features two stages. In the first stage, the strain hardening rate recovers the level before unloading within a relatively small amount of strain. Subsequently, the strain hardening rate decreases faster than it did during the forward loading (Fig. 2d). As a result, the flow stress exhibits permanent softening (Fig. 2c). This type of permanent softening after strain reversal was first observed in [29] for a polycrystalline Al alloy during tension and compression loading and more recently for
Fig. 2. True stress-true strain response under cyclic tension-compression measured along (a) RD and (b) TD. Macro-yield points at approximately 0.001 offset are indicated. (c) True stress-true strain curves as a function of accumulated true strain showing drops in yield stress upon load reversal and permanent softening during subsequent straining. (d) True stress-true strain cyclic curve to a strain of 10% and (e) the corresponding normalized strain hardening rate plots.
the AA6022-T4 alloy during forward and reverse simple shear loading in [77]. This softening was attributed to the annihilation of dislocations (recovery effects) after the reversal of the slip directions during loading in the reverse direction. The difference in the normalized strain hardening behavior in tension vs. compression is clearly evident from Fig. 2e. The normalization factor is the shear modulus, \( \mu \), taken to be 26.1 GPa [84]. The two curves start from the value corresponding to the ratio between Young’s modulus and the shear modulus, \( E/\mu \). Due to non-linear unloading, the compressive curve exhibits drop in strain-hardening rates at zero macroscopic stress. Evidently, the hardening rate is steeper during tensile loading.

Our objective here is to introduce these effects in a crystallographic hardening model which is, in turn, implemented into the polycrystalline EPSC model. The modeling framework is described in the next section.

3. Model description

The EPSC polycrystal model is used for the implementation of the thermally activated dislocation density hardening model featuring forward and reverse motion of dislocations and the slip system kinematic hardening effects. In EPSC, a polycrystal is represented by a set of grains (each having a crystal orientation, an ellipsoidal shape and a volume fraction). Each grain is treated as an elasto-plastic inclusion embedded in a homogeneous effective medium. The effective medium response corresponds to that of the polycrystal and is to be compared with that of the tested sample. Detailed description of the EPSC model can be found in [68, 85, 86]. Here we present the main equations for completeness. In the following description, we use “\( \cdot \)” to represent a contracted or dot product and “\( \otimes \)” for uncontracted or tensor dyadic product.
A linearized relation between homogenized macroscopic stress and strain increments is:

\[ d\sigma = L \, d\varepsilon. \]  

(1)

where \( L \) is the instantaneous elasto-plastic stiffness tensor of the polycrystal matrix. \( L \) is unknown \textit{a priori} and is calculated iteratively using a standard self-consistent procedure [68]. The response of each grain follows from solving the stress equilibrium and compatibility relations for an inclusion embedded in a homogeneous anisotropic matrix under applied loads [68, 87]. The macroscopic and the grain scale stress rate and strain rate are related through the following interaction equation:

\[ d\sigma^c - d\sigma = -L^c \,(d\varepsilon^c - d\varepsilon), \]  

(2)

where \( L^c \) is the effective stiffness given by \( L^c = L \,(S^c - I) \). \( S^c \) is the symmetric Eshelby tensor and \( I \) is the four rank identity matrix. The superscript “c” denotes that a tensor refers to the grain scale physical quantity. Using the above constitutive equations, a localization equation for the strain increment can be derived as:

\[ d\varepsilon^c = A^c \, d\varepsilon, \]  

(3)

where \( A^c = \,(L^c + L^c)^{-1} \,(L^c^* + L) \). \( L^c \) is the crystal instantaneous elasto-plastic stiffness tensor defined later. Increments in polycrystal stress and strain are equal to the volume average of the grain stress increment and strain increments as:

\[ d\sigma = \langle d\sigma^c \rangle \quad \text{and} \quad d\varepsilon = \langle d\varepsilon^c \rangle, \]  

(4)
leading to the following expression: \( L = (L^c A^c) (A^c)^{-1} \). The stress and slip resistances (through the hardening law described later) are updated incrementally for the current deformation step \( n+1 \), with respect to their previously converged values, noted by the superscript \( n \). For example, the new stress of the polycrystalline aggregate is calculated from the overall stress increment, \( d\sigma \), associated with the strain increment, \( d\varepsilon \), using \( \sigma^{n+1} = \sigma^n + d\sigma \).

Following the formulation presented in [70], the driving force (resolved shear stress) for the activation of a slip system is not only influenced by the applied loading (type 1 stresses) and inter-granular stresses (type 2 stresses) originating from the EPSC description of grain interactions, \( m^s \cdot \sigma^c \), but also by the slip system backstress, \( \tau_{bs}^s \). \( m^s \) is the Schmid tensor associated with every slip system \( s \). The Schmid tensor is the unit tensor, defined as the symmetric portion of the dyadic product of two orthogonal unit vectors denoting the slip shear direction and the slip plane normal, respectively. In order for a slip system to be active, it must satisfy the following two conditions: (1) \( m^s \cdot \sigma^c - \tau_{bs}^s = \tau_c^s \), meaning that the resolved shear stress on the \( s \)th slip system has to be equal to the slip resistance reduced for a value of backstress \( (\tau_{bs}^s) \) on slip system (stress needs to be on the single crystal yield surface) and (2) \( m^s \cdot d\sigma^c - d\tau_{bs}^s = d\tau_c^s \), meaning that the \( s \)th slip system has to remain on the evolving single crystal yield surface in a given increment as stress evolves due to hardening. In addition, the formulation allows for only positive shear on a given slip system, i.e., \( \Delta\gamma^s > 0 \), since reverse shear of this slip system would be captured as positive slip on the opposite-signed slip system. The slip systems are defined such that the two slip systems sharing
the same plane normal, but having opposite sense of shear, are independently considered.

The slip resistance and backstress increments are coupled with the shearing increment of the slip systems through the hardening matrices, \( h^{ss'} \) and the backstress matrix, \( h_{bs}^{ss'} \), respectively:

\[
d\tau_c^s = \sum_{s'} h^{ss'} d\gamma^{s'}
\]

\[
d\tau_{bs}^s = \sum_{s'} h_{bs}^{ss'} d\gamma^{s'}
\]

As will be highlighted in the next section, the hardening matrix, \( h^{ss'} \), follows from the hardening law, while the backstress matrix, \( h_{bs}^{ss'} \), follows from the evolution of backstress equations with shear strain.

For the individual grains, the constitutive relation between stress increment \((d\sigma^c)\) and increment in total strain \((d\epsilon^c)\) is:

\[
d\sigma^c = C^c (d\epsilon^c - \sum_s m^s d\gamma^s)
\]

where \( C^c \) is the single crystal elastic stiffness tensor and \( \sum_s m^s d\gamma^s \) is the plastic strain increment calculated as the sum of shear increments, \( d\gamma^s \), over all slip systems per grain. Only slip systems that are active will have non-zero shear increment, \( d\gamma^s \). Similar to the macroscopic stress and strain increments, a linear relationship between grain stress and total strain increment can be written as:

\[
d\sigma^c = L^c d\epsilon^c.
\]
From Eqs. (5, 7, and 8), $L^c$ becomes:

$$L^c = C^c (I - \sum_s m^s \otimes f^s)$$  \hspace{1cm} (9)

where:

$$f^s = \sum_{s'} (X^{-1})^{ss'} m^{s'} C^c.$$  \hspace{1cm} (10)

The matrix, $f^s$, relates an increment in shear strain on individual slip system with the total strain increment in crystal:

$$d \gamma^s = f^s d \epsilon^c$$  \hspace{1cm} (11)

Since the activation condition includes the backstress term, the definition of the $X^{ss'}$ matrix takes the following form:

$$X^{ss'} = h^{ss'} + h_{bs}^{ss'} + m^s \cdot C^c m^{s'}.$$  \hspace{1cm} (12)

For completeness, we briefly reflect on the crystallographic texture evolution calculations in EPSC. In the model, the plastic rotation rate, $W^p$, of each crystal is related to the shear rates on the individual slip systems via the following kinematic formula:

$$W^p = \sum_s \dot{\gamma}^s q^s.$$  \hspace{1cm} (13)

The tensor $q^s$ is the unit slip system tensor, defined as the skew symmetric portion of the dyadic product of two orthogonal unit vectors denoting the slip shear direction and the slip plane normal, respectively. The lattice rotation rate, $W^*$, is calculated as:

$$W^* = W^{app} + \Pi - W^p,$$  \hspace{1cm} (14)
where $W^{app}$ is the macroscopically applied rotation rate of the grain shape and $\Pi$ is the reorientation contribution from the antisymmetric part of the Eshelby tensor [55]. The tensor $W^*$ is used to update the crystal orientation and hence to calculate texture evolution.

### 3.1 Hardening law based on dislocation density

In the present model, the resistance to slip, $\tau_c$, evolves with the rate of dislocation storage, which is governed by thermally activated dislocation glide and hence is dependent on strain rate and temperature. In several prior studies, a similar hardening model has been successfully applied within the self-consistent models to a variety of metals of different crystal structures: hexagonal close packed (HCP) Zr [88-92], Be [73, 93, 94], Mg [95-97], body centered cubic (BCC) Ta [90, 98-101], a face centered cubic (FCC) cobalt alloy [102], and orthorhombic uranium [63, 103, 104]. However, to meet the objectives of this work, we found it necessary to extend the model to include the kinematic hardening at the slip system level and reverse dislocation motion accompanied with the dynamic recovery. Thus, the basic formulation of the hardening model is briefly reviewed.

In the following, the Greek superscript $\alpha \alpha$ represents the $\{111\}\langle110\rangle$ slip family for FCC metals and the superscripts $s$, $s'$ span over the individual slip systems belonging to the family along their arbitrarily chosen positive $s^+$ and negative $s^-$ directions. The resistance to slip is defined as:

$$\tau_c^s = \tau_{0,f}^\alpha + \tau_{0,HP}^\alpha + \tau_{for}^s + \tau_{deb}^\alpha$$

(15)
where $\tau_{0,f}^\alpha$ is a friction stress (dependent on the Peierls stress and the initial content of dislocations), $\tau_{0,HP}^\alpha$ is the Hall-Petch-like term dependent on the initial grain size, $\tau_{for}^s$ is the forest term dependent on statistically stored dislocations, and $\tau_{deb}^\alpha$ is the debris term dependent on amount of dislocations stored as ordered defects.

Effect of grain size on initial slip resistance is modeled using a Hall-Petch-like relation:

$$\tau_{0,HP}^\alpha = \mu_{HP} \sqrt{\frac{b_\alpha}{d_g}}$$

(16)

where $\mu$ is the shear modulus, $HP$ is a Hall-Petch coefficient and $d_g$ is the initial grain size. Note that $\tau_{0,f}^\alpha$ and $\tau_{0,HP}^\alpha$ define the initial slip resistance $\tau_0^\alpha = \tau_{0,f}^\alpha + \tau_{0,HP}^\alpha$ and do not evolve with strain. In the present study the $\tau_{0,HP}^\alpha$ term was not characterized separately but included in the initial slip resistance term, $\tau_0^\alpha$.

Contribution of forest dislocation population to the slip resistance is given by the Taylor relation [88, 105]:

$$\tau_{for}^s = b_\alpha \chi \mu \sqrt{\rho_{tot}^s}$$

(17)

where $b_\alpha = 2.86 \times 10^{-10} m$ is the Burgers vector of the slip mode, $\chi$ is the dislocation interaction constant taken to be 0.9 [106], and $\rho_{tot}^s$ is the total forest dislocation density for the $s^{th}$ slip system ($s \in \alpha$).

Contribution of the dislocation substructures (debris) to the slip resistance is defined through the following relation [107]:

135
\[ \tau_{deb}^\alpha = k_{deb}b^\alpha \sqrt{\rho_{deb}} \log\left(\frac{1}{b^\alpha \rho_{deb}}\right), \]  

(18)

where \( k_{deb} = 0.086 \) is a material independent constant and \( \rho_{deb} \) is the density of dislocations stored as substructure. Justification for the Eq. (18) arises from the basic thermally activated processes such as climb and cross slip, which are responsible for pattern formation [108-111]. Dislocation in these patters self-organize into lower energy patterns, such as cells and cell walls [e.g. 112]. While the hardening model considers these processes to contribute recovery of forest dislocations, it also assumes that a smaller fraction of the recovered forest dislocations contribute to substructure development. The model, however, neglects the length scales associated with substructure. As our present interests lie in modeling cyclic deformation where dislocation cell walls processes take place, advancing the substructure model is left for future work. Evolution of the dislocation densities, \( \rho_{tot}^\text{\&} \) and \( \rho_{deb} \), is described next.

As explained earlier, accurate modeling of the strain-path changes deformation must account not only for the microstructure induced anisotropy during pre-loading, but also for instantaneous rearranging of the microstructure upon reloading in order to predict the change in the initial yield stress and subsequent hardening. An essential element of the developed model is the introduction of reversible dislocations defined as a fraction of the previously stored dislocations that progressively annihilate upon strain reversal. These dislocations, since loosely tangled, re-emit from pile-ups and substructures with very low slip resistance, influencing the hardening behavior upon reloading. An important feature of the model is that it is able to detect the local slip system shear reversal in each grain, which is important since even if the macroscopic
strain is reversed, locally each slip system in each grain may not experience an exact reverse shear.

The total dislocation density is directionally broken into a forward and a reverse on the individual slip systems per grain and explicitly related to the shear activity in each slip system. The approach was implemented within VPSC and successfully applied to capturing the behavior of low carbon steels during strain path changes [28]. In particular, the plateau with low hardening rate present during reloading after large pre-strains was successfully captured.

Several previous studies have shown that during forward deformation of AA6022-T4 dislocations can organize in cell walls, while during loading in the reverse direction existing cell walls dissolve and new cells walls form [113-115]. These microstructural processes are expected to influence the BE and subsequent work hardening. However, a study on strain reversal performed on mild steels [116] found weak to no relationship between the organization of dislocations in cell walls and the mechanical behavior upon strain reversal. These findings were further exploited and reinforced in a combined modeling and experimental study [117], where a reversible dislocation law without an explicit treatment of cell walls was able to predict the BE and work hardening upon strain reversals of several alloys including AA6022-T4, AA1050-O and a low carbon steel.

The directionality in the dislocation based hardening law is introduced as follows. As mentioned earlier each slip system $s$ is split into two systems denoted as $s^+$ and $s^-$ having the same slip plane but opposite slip direction: $\mathbf{b}$ and $-\mathbf{b}$. From this point
onwards, we use superscript $s$ to denote variables that are equal for both slip directions, while $s^+$ and $s^-$ to label variables related to a particular slip direction. The total dislocation density on each slip system consists of:

$$\rho_{tot}^s = \rho^s_{for} + \rho^s_{rev} + \rho_{rev}^s,$$  \hspace{1cm} (19)

where $\rho^s_{for}$ is the forward dislocation density common to both directions $s^+$ and $s^-$ and $\rho^s_{rev}$ and $\rho^s_{rev}$ are the reversible dislocation density populations associated with $s^+$ and $s^-$ directions, respectively.

The dislocation density populations follow laws that depend on previous strain history and shearing direction on slip systems. For the forward dislocation density population, the evolution law is based on the thermal activation [118]:

$$\frac{\partial \rho^s_{for}}{\partial \gamma^s} = (1 - p) \frac{\partial \rho^s_{gen,for}}{\partial \gamma^s} - \frac{\partial \rho^s_{rem,for}}{\partial \gamma^s} = (1 - p) k_1^\alpha \sqrt{\rho^s_{tot}} - k_2^\alpha (\dot{\gamma}, T) \rho^s_{for},$$

$$d \rho^s_{for} = \frac{\partial \rho^s_{for}}{\partial \gamma^s} d\gamma^s$$ \hspace{1cm} (20)

where $k_1^\alpha$ is an adjustable coefficient accounting for rate of generation of statistically stored dislocations, $k_2^\alpha$ is a rate-sensitive coefficient capturing dynamic recovery [88] and $p$ is a reversibility parameter. The latter coefficient, $k_2^\alpha$, is given by:

$$\frac{k_2^\alpha}{k_1^\alpha} = \frac{\chi b^\alpha}{g^\alpha} \left( 1 - \frac{kT}{D^\alpha b^\alpha} \ln \left( \frac{\dot{\gamma}}{\dot{\gamma}_0} \right) \right)$$ \hspace{1cm} (21)

where, $k$, $\dot{\gamma}_0$, $g^\alpha$, and $D^\alpha$ are the Boltzmann constant, a reference strain rate taken to be $10^7$, an effective activation enthalpy and a drag stress, respectively. Dynamic recovery is often associated with thermal activation of dislocation cross-slip and climb, and the
formation of dislocation debris is concomitant with these recovery processes. As a consequence, in the model, the rate of debris development is coupled to the rate of recovery of all active dislocations through:

\[
d\rho_{deb} = \sum \alpha q^\alpha b^\alpha \sqrt{\rho_{deb}} \frac{d\rho_{rem,for}}{dy^s} \bigg|_{dy^s}
\]  

(22)

where \( q^\alpha \) is a dislocation recovery rate coefficient defining the fraction of \( \alpha \)-type dislocations that do not annihilate but become debris.

The reversibility parameter divides increments in the total dislocation density \( (k_1^\alpha \sqrt{\rho_{tot}} dy^s) \) into: the forward \( ((1 - p)k_1^\alpha \sqrt{\rho_{tot}} dy^s) \) and the reversible \( (pk_1^\alpha \sqrt{\rho_{tot}} dy^s) \). The value of the reversibility parameter is taken to be unity, meaning that all statistically stored dislocation densities are reversible, which is suggested in [28] to be a good approximation up to pre-strains of 0.3. While the evolution of the forward dislocation population, \( \rho_{for}^s \), is independent on the shearing direction on a slip system, the reversible dislocations populations evolve with a particular direction of shearing. If the direction of shearing is positive, \( dy^{s+} > 0 \), then the law is as follows:

\[
\frac{\partial \rho_{rev}^s}{\partial y^{s+}} = pk_1^\alpha \sqrt{\rho_{tot}} - k_2^\alpha (\dot{\varepsilon}, T) \rho_{rev}^s,
\]  

(23a)

\[
\frac{\partial \rho_{rev}^s}{\partial y^{s+}} = -k_1^\alpha \sqrt{\rho_{tot}} \left( \frac{\rho_{rev}^s}{\rho_0^s} \right)^m,
\]  

(23b)

where \( m \) is the parameter taken to be 0.5 controlling rate of dislocation recombination [72] and \( \rho_0^s \) is the total density that was present when the shear was reversed on the \( s^{th} \) slip system [28]. The relation for decay of reversible dislocation densities with shear strain, 23b, was proposed and physically justified in [28, 117], but without parameter \( m \),
which was added in [72] to increase rate of dislocation recombination at the start of reversal and decrease the rate towards the end of reversal. The underlying physical justification for Eq. (23b) is that the rate of recombination of dislocations moving backward is limited by the storage rate they had when moving forward and that the process of recombination decreases and vanishes with \( \rho_{rev}^s \). If shearing occurs in the negative direction, \( dy^s_\neg > 0 \), the increment assigned to \( \rho_{rev}^s \) evolution is analogous to that presented in (23a), while the increment assigned to \( \rho_{rev}^s \) evolution is equal to that of (23b). The initial conditions for the dislocation population evolution laws are: \( \rho_{for}^s(y^s = 0) = \rho_{initial}^s, \rho_{rev}^s(y^s = 0) = 0 \) and \( \rho_{rev}^s(y^s = 0) = 0 \). The initial dislocation density, \( \rho_{initial}^s \), was initialized to a small value of \( 10^{12} \) m\(^{-2} \).

Based on Eq. (5), the evolution of the resistance on a slip system is done via instantaneous hardening coefficients \( h_{ss'} \). Current slip resistance, \( \tau_c^s \), on a slip system \( s \) is a function of dislocation densities (\( \rho_{for}^s \) and \( \rho_{deb}^s \)), which are in turn the function of the shearing strain on slip systems inside crystal (\( y^s \)). This implies that we must evaluate:

\[
h_{ss'} = \frac{\partial \tau_c^s}{\partial y^{s'}} ,
\]

(24)

which can be further expanded to:

\[
\frac{\partial \tau_c^s}{\partial y^{s'}} = \frac{\partial \tau_0^s}{\partial y^{s'}} + \frac{\partial \tau_{for}^s}{\partial y^{s'}} + \frac{\partial \tau_{deb}^s}{\partial y^{s'}} + \frac{\partial \tau_{0,HP}^s}{\partial y^{s'}} .
\]

(25)

Using the chain rule and based on the above equations, individual terms from equation (25) evaluate to:

\[
\frac{\partial \tau_0^a}{\partial y^{s'}} = \frac{\partial \tau_{0,HP}^a}{\partial y^{s'}} = 0 .
\]
\[
\frac{\partial \tau_{for}^s}{\partial y^{st}} = \frac{\partial^2 \tau_{for}^s}{\partial \rho_{tot}^s \partial y^{st}} = b^\alpha \chi \mu \frac{1}{2 \sqrt{\rho_{tot}^s}} \left( \frac{\partial \rho_{for}^s}{\partial y^{st}} + \frac{\partial \rho_{reg}^s}{\partial y^{st}} + \frac{\partial \rho_{rev}^s}{\partial y^{st}} \right), \text{ if } s = s' \text{ else } \frac{\partial \tau_{for}^s}{\partial y^{st}} = 0,
\]

\[
\frac{\partial \tau_{deb}^s}{\partial y^{st}} = \frac{\partial^2 \tau_{deb}^s}{\partial \rho_{deb} \partial y^{st}} = -k_{deb} \mu b^\alpha \left[ \log \left( b^\alpha \sqrt{\rho_{deb}} \right) + 1 \right] \frac{1}{2 \sqrt{\rho_{deb}}} \frac{\partial \rho_{deb}}{\partial y^{st}}.
\] (26)

3.2 Evolution law for backstresses

As mentioned earlier, the introduction of kinematic hardening is necessary for capturing the micro plasticity processes responsible for non-linear unloading and the BE. In order for crystals to start micro-yielding, the following condition has to be fulfilled: \( \mathbf{m}^s \cdot \mathbf{c}^c - \tau_{bs}^s = \tau_c^c \). Satisfying this condition is controlled in part by evolution of the backstresses. Here, we extend the EPSC model to account for the effect of intra-granular micro backstresses at the slip system level.

Several evolution laws for backstress with shear strain have been proposed in the literature. The Armstrong and Frederick model [33] has been adopted in crystal plasticity and successfully employed in several prior studies [119–121]. Another phenomenological law for the evolution of backstress based on a modified Voce hardening law was used to simulate the cyclic deformation of stainless steel [70]. However, these studies dealt with small pre-strains (~0.02) and multiple cycles. A model for the evolution of backstress based on experimental observations [122] applicable to large pre-strains has been presented in [71]. The model was successfully applied in VPSC to pre-strains of 0.08, 0.18 and 0.28 followed by reloading. We adapt this model for the evolution of backstress in the present study dealing with large pre-strains in EPSC.
Fig. 3. Schematics showing (a) a given slip system $s$ split into $s^+$ and $s^-$ under action of the directional micro backstresses formed during slip in the $+b$ direction ($d\gamma^{s^+} > 0$), (b) the long range micro backstresses acting on the dislocations that are primary mobile during forward loading and (c) the near pile-up micro backstresses acting on the dislocations that are primary mobile during unloading.

The origin of backstresses in Al alloys is the stress field arising from dislocation loops formed around precipitates [123]. When a dislocation surpasses a non-shearable obstacle such as a precipitate particle present in Al alloys [115, 124], it leaves a dislocation loop around it. During plastic deformation, dislocation loops keep accumulating around the precipitates and the backstress field strengthens [123, 125]. Thus evolution of the backstresses is directly proportional to the number of dislocation loops formed around precipitates. Analogous expression for the evolution of the number of dislocation loops to the law adopted here from [71] for the evolution of backstresses with shear strain has been suggested in [123], which justifies the use of the backstress law for precipitation hardened alloys.
In what follows, the evolution laws for the slip system backstresses are described during the course of forward loading (pre-strain) and unloading followed by reverse loading. Schematic illustration defining direct and opposite slip systems $s^+$ and $s^-$ under the micro backstresses is shown in Fig. 3.

### 3.2.1 Evolution of backstresses during forward loading

Similarly to the directional definition of reversible dislocation, the backstresses associated with each slip system are defined directionally. We recall that each slip system is divided into two systems $s^+$ and $s^-$ having the same slip plane normal $n$ but opposite slip directions: $b$ and $-b$ which is illustrated in Fig. 3a. If the direction of shearing is positive, $d\gamma^{s^+} > 0$, then the evolution of backstresses is governed by the following law:

\[ \tau_{bs}^{s^+} = \tau_{bs}^{sat} (1 - \exp(-\nu \gamma^{s^+})) , \]  
\[ \tau_{bs}^{s^-} = -A \tau_{bs}^{s^+} \]  

(27a)  
(27b)

where $\tau_{bs}^{s^+}$ and $\tau_{bs}^{s^-}$ are backstresses in the two opposite directions per slip system, $\tau_{bs}^{sat}$ is a saturation value for backstresses, $A$ and $\nu$ are adjustable material parameters and $\gamma^{s^+}$ is the accumulated value of shear strain on that slip system.

The slip system backstress $\tau_{bs}^{s^+}$ acts in the direction which is opposite to the resolved shear stress on that slip system (Fig. 3b). Therefore, $\tau_{bs}^{s^+}$ lowers the activation stress i.e.: $m^{s^+} \cdot \sigma - \tau_{bs}^{s^+} = \tau_{c}^{s^+}$. At the same time, $\tau_{bs}^{s^+}$ acts in the direction of resolved shear stress on the slip system $s^-$ meaning that the backstress on the $s^-$ system is of the opposite sign i.e. $\tau_{bs}^{s^-} = -\tau_{bs}^{s^+}$. Therefore, $\tau_{bs}^{s^-}$ aids the resolved shear stress according
to: \( \mathbf{m}^{s^-} \cdot \sigma^c - \tau_{b_s}^{c^-} = \tau_{c^-}^{s^-} \). However, the backstress acting on the slip system \( s^- \) is much higher than on the slip system \( s^+ \). We now turn our attention to a physical justification of the scaling parameter \( A \) in Eq. 27b.

During forward loading majority of plastic deformation is accommodated by the dislocations that are under long-range internal stresses, while a much smaller portion of plastic strain is accommodated by decreasing spacings between the dislocations in a pile-up (Fig. 3b). Upon local unloading, the dislocations in a pile-up mobilize because stress acting on them in the forward direction decreases (Fig. 3c). With the unloading process, dislocation pile-ups expand accommodating some micro shear strain in the reverse direction. Driving force for these processes are believed to be the micro backstresses of high magnitude arising from pile-ups [6]. We relate these micro backstresses to the long range backstresses by parameter \( A \). Dislocation pile-ups also contribute to the long range stresses [19, 23, 126], therefore relating the pile-up micro backstresses to the long range backstresses is plausible. Dislocations re-emitted from pile-ups are believed to experience significantly lower resistance to their motion in the backward direction [6]. Therefore, justification for a large value of the parameter \( A \) is twofold: (1) the large micro backstress arising from pile-ups and (2) the low resistance to slip of dislocations re-emitted from pile ups. The predicted value for \( A \), based on our model, is \( \sim 10 \).

3.2.2 Evolution of backstresses upon unloading followed by reverse loading

As mentioned earlier, the physical origin of nonlinear unloading is in the short range motion of dislocations re-emitted from pile-ups under action of the micro backstresses that have a large magnitude [6, 127]. During unloading these micro
backstresses relax while pile-ups expand giving rise to a micro plastic strains in the reverse direction \((d\gamma_s^- > 0)\). The slip system \(s^-\) can continues to be active after the local micro backstresses relax due to action of the applied stress in the reverse direction (type 1 stress). To this end, an evolution law for \(\tau_{bs}^{s^-}\) must capture: (1) a rapid nullification followed by (2) a saturation type evolution law in the reverse direction. The saturation value for \(\tau_{bs}^{s^-}\) is conveniently chosen to be the backstress at the point of strain reversal \([27, 71, 122]\). An appropriate evolution law for \(\tau_{bs}^{s^-}\) during unloading followed by loading in the reversed direction, which fulfills the above defined conditions, is expresses as:

\[
\tau_{bs}^{s^-} = -(A + 1)\tau_{bs0}^{s+} \exp\left(-\frac{\gamma_s^-}{\gamma_b}\right) + \tau_{bs0}^{s+} \quad (28a)
\]

\[
\tau_{bs}^{s+} = -A\tau_{bs}^{s-} \quad (28b)
\]

where \(\tau_{bs0}^{s+}\) is the value of backstress at the point of the strain reversal and \(\gamma_b\) is another adjustable material parameter. Eq. (28a) evolves \(\tau_{bs}^{s-}\) with accumulated shear strain \(\gamma_s^-\), from an initial value of \(-A\tau_{bs0}^{s+}\) to a new saturation value conveniently chosen to be the backstress at the point of reversal. Note that \(s^+\) is now inactive and that \(\tau_{bs}^{s+}\) and \(\tau_{bs}^{s^-}\) are related using the same parameter \(A\) as used in Eq. 27.

Based on Eq. (6), the evolution of the backstress on a slip system is done via instantaneous hardening coefficients \(h_{bs}^{s^s'}\) defined as:

\[
h_{bs}^{s^s'} = \frac{d\tau_{bs}^{s^s'}}{d\gamma_s} = \tau_{bs}^{sat} \nu \exp(-\nu\gamma_s^s) \quad (29)
\]

\[
h_{bs}^{s^s} = \frac{d\tau_{bs}^{s^s}}{d\gamma_s} = \frac{(A + 1)\tau_{bs0}^{s^+} \exp\left(-\frac{\gamma^s}{\gamma_b}\right)}{\gamma_b} \quad (30)
\]
where \( s \) span over the available slip systems in positive, \( s^+ \), and negative, \( s^- \), directions. The off diagonal terms evaluate to zero.

In the next section, this model is used to predict the cyclic stress-strain response of the polycrystalline AA6022-T4 alloy. We calibrate and critically validate the model against the experimental data presented in section 2 and provide insights into the effect of the residual stresses, backstresses, and reversible dislocations on various aspects of the elasto-plastic material response during cyclic loading to large pre-strains.

4. Results and discussion

We represent the initial texture (Fig. 1b) of the material using 1000 weighted orientations and assign an initially spherical shape to the representative ellipsoids. Loading in cyclic tension and compression was simulated by imposing strain increments along RD or TD, while enforcing zero average stress along the lateral two sample directions. As deformation proceeds, grains are allowed to change their crystal orientation and shape to become ellipsoids.

4.1 Calibration of parameters

We compared simulated and measured 10% tensile true stress-true strain curves to determine the following slip system material parameters: initial slip resistance, \( \tau_0^\alpha \), trapping rate coefficient, \( k_1^\alpha \), activation barrier for de-pinning, \( g^\alpha \), and drag stress, \( D^\alpha \). Each of these parameters affects different portions of the stress-strain curve. For example, \( \tau_0^\alpha \) is responsible for the yield stress and \( k_1^\alpha \) mainly governs the initial slope of the stress-strain curve. Consequently, it is possible to obtain a reasonable estimate of these parameters even from one stress-strain curve. To establish the kinematic
backstress parameters, we utilized the entire 10% cyclic curve. The parameters were only slightly corrected to better fit the RD 2% cyclic curve. The corresponding set of parameters is given in Tables 1 and 2. The remaining experimental cyclic curves were used to test the model’s predictive capabilities with this set. The comparison of the model (dash) and experimental curves (solid) is given in Fig. 4.

**Table 1.** Constitutive parameters for evolution of slip resistance.

<table>
<thead>
<tr>
<th>$\tau_0^\alpha [MPa]$</th>
<th>$k_1^\alpha [m^{-1}]$</th>
<th>$q^\alpha$</th>
<th>$D^\alpha [MPa]$</th>
<th>$q^\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>51</td>
<td>2.1x10^8</td>
<td>0.02</td>
<td>2500</td>
<td>16</td>
</tr>
</tbody>
</table>

**Table 2.** Parameters for evolution of kinematic hardening.

<table>
<thead>
<tr>
<th>$\tau_{bs}^{sat}$</th>
<th>$v$</th>
<th>$y_b$</th>
<th>$A$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>60</td>
<td>0.0008</td>
<td>10</td>
</tr>
</tbody>
</table>

4.2 Predictions of mechanical response

From the comparison between simulated and measured curves, it is evident that the model is capable of predicting all of the particularities associated with cyclic tension-compression deformation of the AA6022-T4 alloy.

We observe that the flow stresses and hardening rates during monotonic tension are well captured. The tensile curve exhibits a classical decreasing hardening rate throughout. Upon strain reversal, the model remarkably captures non-linear unloading as well as the drop in yield stress. Subsequently, there is a more pronounced decrease in hardening rate during compression in the reverse direction due to the annihilation of loosely tangled dislocations. The model captures this shift in the hardening rate. Finally, to explore plastic anisotropy, cyclic tests were simulated in the transverse direction.
Figure 4b reveals a small plastic anisotropy between RD and TD attributed to the initial crystallographic texture.

Fig. 4. Measured and simulated true stress–true strain response of AA6022-T4 samples in cyclic tension-compression along (a) RD and (b) TD. The solid lines are the experimental curves and the dashed lines are the model calculations.

A key achievement of this work is that the model is shown to provide very good agreement for all cyclic stress-strain responses using a single set of parameters. Specifically, the small plastic anisotropy, hardening rates, non-linear unloading, BE and permanent softening are simultaneously captured. As many of these features in flow stress of AA6022-T4 are similar to those in other cubic metals, the present modeling framework is expected to be useful for a wider set of materials in addition to Al alloys.

Good predictions of the cyclic mechanical behavior were the result of a combination of three distinct mechanisms incorporated in the model. The inter-granular
Fig. 5. Measured and simulated true stress–true strain response of AA6022-T4 samples in cyclic tension-compression along RD (a) without residual stresses, (b) without backstresses, (c) without residual and backstresses, and (d) without reversible dislocations. The solid lines are the experimental curves and the dashed lines are the model calculations.

residual stresses, backstresses, and reversible dislocations mechanisms were all active in the simulations. To isolate the individual contribution of these mechanisms on the material response during cyclic loading, we performed the RD simulations without the
contributions of (a) the residual stresses, (b) the backstresses, (c) the residual stress and backstresses, and (d) the reversible dislocations. The effects are shown in Fig. 5.

4.2.1 Effect of residual stress

Figure 5a shows experimental results together with the EPSC predictions without consideration of the residual stresses upon reloading. From the comparison between Fig. 4 and Fig. 5a, it is evident that inter-granular residual stresses are aiding plastic deformation in the opposite direction (in this case the compression). To more clearly illustrate the effect of the inter-granular residual stress on subsequent loading, we compare the material response after continuous deformation in tension and in compression in Fig. 6. The starting point of the continuous deformation is the unloaded state, i.e. zero overall macroscopic stresses (type 1 stresses). Thus, during subsequent loading, only type 1 stresses contribute to the left hand side of the activation condition for the slip systems ($\mathbf{m}^s \cdot \sigma^c = \tau^s_c$). With inter-granular residual stresses (the type 2 stresses) being erased, the model predicts a decrease in yield stress in tension as well as in compression compared to that at the end of tension (the difference is around 40 MPa). In this case, both the tensile and the compressive yield stresses are the same (the response is symmetric). This is because the response is controlled by the slip resistance, $\tau^s_c$, recorded at the end of tension pre-straining. In contrast, when the inter-granular stresses are present, the response is asymmetric. While the yield stress in tension returns to the original value upon continued loading, the yield stress in compression drops more. This behavior is due to the inter-granular residual stresses that are “aiding” the deformation in reverse direction. The difference in yield stress in
compression vs. tension comes from the left hand side of the activation law reflecting the stress state in grains.

Fig. 6. Effect of residual stresses on material response upon reloading in forward and reverse directions.

The effect of residual stress on the shift in yield stress in compression is more significant at larger pre-strains. The similar effects of residual stress on the cyclic deformation were also reported in [119], where an analysis of the effect of residual stress was performed at small pre-loads. Additionally, strong effects of the residual stresses on the material response of an AA6111 aluminum alloy after pre-straining have
been highlighted in [128]. Interestingly, residual stresses do not play a major role for the non-linear unloading (Fig. 5a).

4.2.2 Effect of backstresses

Figure 5b compares measured stress-strain curves predicted with the model without consideration of the backstresses. To ensure as fair comparison as possible, the material parameters were readjusted. Table 3 shows the new material parameters used in the simulations without consideration of the backstresses. Evidently the backstresses are responsible for the early yielding upon reloading and rapid hardening that follows. These conclusions are in good agreement with prior works [27, 71, 122]. In their analysis on Cu [71], the backstresses reached their maximum value between 0.05 and 0.1 true strain in forward loading. Upon the strain reversal, the backstresses are predicted to decay rapidly, ending at approximately 0.01 true strain [71]. In the study done on low- and high-carbon steels in [122], backstresses were estimated using the X-ray diffraction technique. Results of measurements showed that backstresses increase rapidly to approximately 0.03 true strain and continue to grow between 0.05 and 0.1 true strain with lower rate. After reversal the backstresses quickly decay and grow in the reverse direction reaching approximately 80% of their maximum value by 0.05 strain. Similarly to [71] they found that backstresses were nullified within 0.02 reverse strain. In our analysis, the model predicts that backstresses rapidly increase to approximately 0.05 true strain and then slowly saturate at approximately 0.15 true strain, while in the opposite direction the backstresses are erased by 0.01 true strain and rapidly grow.
Table 3. Constitutive parameters for evolution of slip resistance (without backstresses).

<table>
<thead>
<tr>
<th>$\tau_0^0$ [MPa]</th>
<th>$k_{1}^\alpha [m^{-1}]$</th>
<th>$q^\alpha$</th>
<th>$D^\alpha [MPa]$</th>
<th>$q^\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>51</td>
<td>3.7x10^8</td>
<td>0.012</td>
<td>1500</td>
<td>16</td>
</tr>
</tbody>
</table>

4.2.3 Combined effect of residual stress and backstresses

Figure 5c shows experimental results together with the EPSC calculations performed without consideration of the backstresses and residual stresses. These simulations were performed with the parameters reported in Table 3. We observe that the non-linear unloading is not well captured, suggesting that the backstresses are mainly responsible for capturing the non-linear unloading effects.

4.2.4 Effect of reversible dislocations

Figure 5d shows experimental results together with the EPSC calculations performed without consideration of reversible dislocation. The total dislocation density consisted of only forward dislocations. These simulations were performed with the parameters reported in Tables 1 and 2. It is evident that without reversible dislocations the model is unable to predict the work hardening after reversal. It also should be noted that the effect of reversible dislocations on the predictions of the BE is minimal. Figure 7 shows a comparison between the evolutions of the total dislocation density during the cyclic tension-compression simulations in RD with and without consideration of the reversible dislocations. The results indicate that after the strain reversal a certain amount of plastic strain can be accumulated without a marked increase in total dislocation density. These results are in agreement with the constitutive assumption made to develop cyclic plasticity models in [129, 130].
After the above analysis and interpretation, we can more confidently discuss the mechanism governing the cyclic response of the AA6022-T4 alloy. We infer first that the backstresses have a dominant effect on non-linear unloading, next that the intergranular residual stresses and backstresses control the BE, and finally that the inclusion of reversible dislocation motion is the key for capturing the hardening rates during reverse loading. As these effects have major implications on the accuracy of numerical simulations of forming processes, they must be captured by the constructive laws used in such simulations. The good predictions by the present model represent a significant incentive for incorporating the model into finite-element (FE) frameworks to facilitate treatment of complex, non-monotonic deformation processes with heterogeneous boundary conditions. The resulting FE-EPSC model would couple sensitivity of microscopic mechanisms to complex macroscopic changes of imposed strain paths.
5. Conclusions

In this paper we presented a polycrystal plasticity model able to predict elasto-plastic cyclic tension-compression deformation behavior of metals to large plastic strain levels. The model is based on the self-consistent homogenization of single crystal responses and allows for a detailed comparison with macroscopic measurements. The performances of the developed model were tested on a data set collected for the AA6022-T4 sheets under in-plane cyclic deformation. The stress-strain response of the material exhibited the typical decreasing hardening rate in forward tensile deformation. The reverse deformation of the material started with linear and then non-linear unloading, followed by the transient Bauschinger effect, which is characterized by the early yielding and rapid increase in the work hardening rate. Finally, deformation during continuous loading in the reverse direction showed a decrease in the work hardening rate resulting in permanent softening. The latter indicated that the work hardening rate is larger during forward than during reverse loading.

To model the cyclic response of the material, the following main extensions to the EPSC model were implemented:

1. a kinematic hardening law at the slip system level able to capture the non-linear unloading behavior and the BE.
2. a dislocation density based hardening law that evolves the slip resistance while accounting for the forward and reverse glides. To predict the hardening behavior during loading in the reverse, the formulation models instantaneous rearrangement of the microstructure upon reloading, and progressive annihilation of dislocation during continuous loading in the reverse direction.
It was shown that the model successfully explains the flow response of the material during cyclic tension-compression deformation to large plastic pre-strains. Specifically, the plastic anisotropy, hardening rates, non-linear unloading, BE and permanent softening were simultaneously captured using a single set of material parameters. As many of these features in flow stress of AA6022-T4 are similar to those in other cubic metals, the present modeling framework is expected to be useful for a wider set of materials in addition to Al alloys.

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CHAPTER 5:

Latent hardening within the elasto-plastic self-consistent polycrystal homogenization to enable the prediction of anisotropy of AA6022-T4 sheets

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Latent hardening within the elasto-plastic self-consistent polycrystal homogenization to enable the prediction of anisotropy of AA6022-T4 sheets

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Abstract

Slip system hardening behavior of a given slip system is influenced more by shearing on another slip system known, as latent hardening, than by shearing on itself, known as self-hardening. This paper extends a recently developed dislocation-based hardening law within the elasto-plastic self-consistent polycrystal plasticity model to incorporate the latent hardening effects for predicting anisotropic response of polycrystalline face-centered cubic metals. In doing so, a new approach to overcome singularities associated with the self-consistent Eshelby solution procedure is proposed. The new approach is validated using a regularized Schmid law, where the singularity in Eshelby tensor calculation is intrinsically suppressed. Moreover, the solution procedure for single crystal stress increment is advanced to be based on a methodology involving the singular value decomposition and a penalty method to solve for shear increments and a set of active slip systems, respectively. It is found that modeling crystallographic
texture evolution and latent hardening successfully captures the anisotropic behavior of polycrystalline AA6022-T4 alloy. The model is subsequently successfully applied to predict large strain cyclic deformation of the same material. The implementation and insights from these predictions are presented and discussed in this paper.

*Keywords*: A. Microstructures; B. Crystal plasticity; B. Polycrystalline material; C. Numerical algorithms; AA6022-T4
1. Introduction

Anisotropy in flow stress of Al and Al alloys has been thoroughly studied, and several possible sources of anisotropy have been identified in the literature, including an initial texture and texture evolution, precipitate shape and orientation, dislocation cell structure formation, and latent hardening. Experimental observations suggested that the anisotropic hardening behavior could result mostly from crystallographic texture evolution. For instance, a study on anisotropy exhibited by commercially pure Al (AA1050-O) suggested that initial texture and texture evolution was the main reason for anisotropy [1]. The shape and direction of precipitates was related to plastic anisotropy in Al-Si-Mg alloys [2] and in Al-Cu alloys [3]. These alloys contain precipitates that are larger in size meaning that they are not shearable. Therefore, their effect was analyzed by assuming that they are inclusions inside the matrix [4]. The backstress in matrix was defined based on the stress in the precipitates, since the volume average of backstress over matrix and precipitates vanishes. However, the effect of precipitates on anisotropy in the AA6022-T4 is not expected to be high because these precipitates are small in size and shearable by mobile dislocations. Studies on pure Al [5] as well as on the alloys with very small shearable precipitates showed that texture alone is not enough to explain the anisotropy. Predictions based on texture sensitive crystal plasticity models often over predict hardening anisotropy compared to experimental measurements [6]. Another study revealed that the formation of dislocation cell structures was a major source of anisotropic hardening in AA1050-O, particularly during strain path change deformation [7]. While AA1050-O was found to develop a well-defined dislocation microstructure during deformation, predominantly dislocation walls on the \{111\} planes,
the AA6022-T4 alloy develops primarily uniform dislocation distribution displaying some walls, which are very faint [8]. Thus, the effect of substructure on anisotropy of AA6022-T4 was suggested to be minimal. The effect of latent hardening and dislocation interactions on plastic anisotropy evolution using crystal plasticity was investigated in [9], where a solid solution strengthened alloy without precipitates is examined. The general trends were successfully explained by latent hardening.

Slip system hardening behavior of a given slip system is complex because it is influenced more by shearing on another slip system, known as latent hardening, than by shearing on itself, known as self-hardening [10]. Additionally, the slip resistance increases not only on the active but also on the inactive slip systems. The latent hardening was documented first for single crystal in [11]. The single crystal latent hardening experiments can be conducted as follows: first, a single crystal is deformed to activate a single slip system, termed as the primary slip system. Next, the loading is changed with respect to the initial crystal orientation to activate another slip system, termed as the secondary slip system. The evolution of slip resistances on primary and secondary slip systems can be inferred from the stress strain measurements [10, 12, 13]. Two theories of latent hardening can be found in the literature [14]. These theories are schematically presented in Fig. 1. Accordingly, yielding of secondary slip system is defined by: the back-extrapolated yield stress [10, 15, 16] (hereafter referred to as “theory 1”) and the elastic limit [14, 17, 18] (hereafter referred to as “theory 2”). The former is obtained by back-extrapolation using the initial hardening slope, $\theta$, of the stress-strain curve recorded during the activation of secondary slip system, to the end of the stress-strain curve of the primary slip system [13]. Theory 1 view on latent
hardening is grossly predominant in the literature and is supported with a large body of studies performed since 1960s, hence it is termed as theory 1, while the more recently proposed theory of Bassani and Wu in 1991 is termed as theory 2.

**Fig. 1.** Schematic showing hardening of the secondary slip system \( s = 10 \) due to shearing on the primary slip system \( s = 4 \) according to the elastic limit theory of yielding \( \tau_{e}^{10} \) and the back-extrapolated theory of yielding \( \tau_{be}^{10} \). Shear strain and resolved shear stress are plotted on the x-axis and the y-axis, respectively. The slip systems are labeled according to commonly used notation for FCC metals from [19].

In theory 1 the shear strain on a given slip system leads to an increase in slip resistance of all slip systems, which can be mathematically expressed as:

\[
\tau_{be}^{s} = \tau_{be}^{s}(\gamma^{1}, \gamma^{2}, ..., \gamma^{n}); \ h^{ss'} = \frac{\partial \tau_{be}^{s}}{\partial \gamma^{s'}} = f(\gamma^{1}, \gamma^{2}, ..., \gamma^{N}).
\]  

(1)

where \( \tau_{be}^{s} \) is the slip resistance based on the back-extrapolated yield stress and the matrix of partial derivatives of slip resistance with respect to shear strain, \( \frac{\partial \tau_{be}^{s}}{\partial \gamma^{s'}} \), is hardening matrix. Entries of the hardening matrix are also referred to as the hardening moduli or instantaneous moduli. We note that according to theory 1, hardening matrix is
predicted to have off diagonal terms. The added advantage of theory 1 is that it is possible to define a law for the evolution of slip resistance and then derive the corresponding hardening matrix. Therefore, the focus in theory 1 is on slip resistance, while the hardening matrix is defined by partial derivatives with respect to shear strain.

Experimental data presented in [17] formed basis for the development of theory 2 [12]. In this theory, the rate of hardening \( h_{ss}(\gamma^1, \gamma^2, \gamma^3, \ldots \gamma^N) \) of a given slip system \( s \) depends on shearing on itself \( F(\gamma^s) \) and shearing on all the other slip systems \( G(\gamma^{st}; s' = 1 \ldots N, s' \neq s) \), i.e. the rate of hardening is the product of \( F \) and \( G \) \( (h_{ss} = FG) \). However, the slip resistance of a given slip system \( s \) increases primarily due to shear strain (activity) on that slip system because the hardening matrix is diagonal or diagonal dominant i.e., \( h_{ss} \gg h_{ss'} \). Neglecting the small off-diagonal terms for the case of diagonal dominant hardening matrix, theory 2 can be mathematically expressed as:

\[
d\tau_e^s = h_{ss} \, d\gamma^s; \quad h_{ss} = f(\gamma^1, \gamma^2, \ldots \gamma^N); \quad h_{ss'} = 0
\]  

(2)

where \( \tau_e^s \) and \( \gamma^s \) are slip resistance based on the elastic limit, shear strain on \( s^{th} \) slip system, and \( N \) is the total number of slip systems. The focus is on the hardening rate. Intrinsic to this theory is that it evolves hardening rate while keeping the slip resistance constant until the activation happens, when the hardening takes place to increase the slip resistance.

The response of a polycrystal depends on the constituent single crystals, whose response is affected by latent hardening. The response of single crystals undergoes homogenization to represent the overall behavior of a polycrystalline metal. Homogenization schemes such as upper bound Taylor-type [20-25], mean-field self-
consistent (SC) [26-28], full-field finite element [29-38], and Green’s function-based fast Fourier transforms [39, 40] are most widely used. The SC homogenization approach is the most widely used because it provides the best compromise between computational speed and accuracy.

A number of polycrystal plasticity models consider both self and latent hardening [30, 41-45]. Both self and latent hardening are included in the latent hardening matrix, which is also called the interaction matrix. The matrix describes the relative strength of various dislocation interactions. These interactions can be similar for a wide range of alloys with the same crystal structure. The latent hardening coefficients are most often calibrated to fit multiple stress-strain curves of a studied material. The values in the matrix can also be measured experimentally [10, 13, 46, 47] or calculated using dislocation dynamics [48-50].

Numerical issues with the incorporation of latent hardening in crystal plasticity models have been observed in literature [15, 51]. Specifically, the incorporation of the theory 1 of latent hardening in the elasto-plastic self-consistent (EPSC) formulation [52] of interest in the present work requires the development of a new approach due to the singularities arising from the SC Eshelby solution procedure. Moreover, the solution procedure for single crystal stress increment needs to be advanced. The objectives of the present paper are to: (1) enable a crystallographic hardening law within EPSC homogenization [53, 54] to consider the physics of latent hardening, (2) reveal the origin of plastic anisotropy in AA6022-T4 by modeling the effects of latent hardening, and (3) predict the characteristics of large strain cyclic deformation for the material.
2. Material

This study is carried out on AA6022-T4 alloy, which is an important age-hardenable aluminum alloy exhibiting an excellent combination of strength and ductility [55]. The typical chemical composition of the alloy in wt. % is 1.21 Si, 0.56 Mg, 0.12 Fe, 0.08 Mn, and 0.05 Cu, balanced with Al. The AA6022 alloy can have a certain amount of precipitates, depending on the aging treatment [2, 56, 57]. The precipitates, together with solutes, impede dislocation motion [7]. Since AA6022-T4 does not undergo artificial aging, the content of precipitates is small. The response is measured in simple tension along the rolling direction (RD), at 45° with respect to RD, and the transverse direction (TD) [58, 59]. Several tests were carried out per test direction and the recorded curves were within a spread of 2 %. The alloy exhibits a classic decreasing hardening rate, which is similar to many materials deforming by crystallographic slip. Evidently, the plastic anisotropy evolves with plastic strain. The r-ratio, defined as the ratio between the in-plane plastic strain in the direction perpendicular to the loading direction and the plastic strain in the through-thickness normal direction (ND), is plotted as a function of plastic strain in the loading direction in Fig. 2b.

The initial crystallographic texture of the alloy was measured using electron backscattered diffraction (EBSD) over a large area and is shown in Fig. 2c using the pole figures visualization. It predominantly contains a cube texture component spread of moderate intensity. The average grain size in the material is estimated from EBSD scans to be approximately 44 μm.
Fig. 2. Mechanical response and initial texture of AA6022-T4 alloy: (a) true stress-true strain response in simple tension along RD, TD, and at 45° with respect to RD, (b) evolution of r-ratio with plastic strain during simple tension along RD, TD, and at 45° with respect to RD, (c) pole figures showing the initial texture, and (d) large strain cyclic tension-compression response measured along the RD.
The alloy was also tested under the cycle tension-compression along the RD to four levels of true strain: 0.01, 0.05, 0.1 and 0.15 (Fig. 2d), as reported in [60]. The testing setup for acquiring such data was explained in our earlier work [54]. The macroscopic characteristic of the alloy behavior upon unloading is the existence of a very short initial linear portion followed by a larger non-linear unloading portion, which is further followed by a drop in yield stress relative to that reached at the end of forward straining. The phenomenon is known as the Bauschinger effect (BE) [61]. Subsequently, the hardening rate in compression is different from the hardening rate during forward tension. As a result, the alloy exhibits what is known as the permanent softening behavior [62], which is governed by the annihilation of dislocations during compression in the reverse direction.

3. Elasto-plastic self-consistent formulation

The modeling framework presented in this work is intended for understanding material behavior and simulations of metal forming, which subject metals to large plastic strains developing highly non-uniform stress-strain fields [59, 63-69]. These fields are intra- and inter-granular heterogeneities and play a significant role during strain-path changes and unloading [61, 70, 71]. The EPSC model was originally developed in [52, 72, 73]. Below, we provide a summary of the EPSC model.

In the description that follows, “•” will represent a dot product, “⊗” will represent a tensor product, and α will be used to denote a family of slip systems while s will denote individual slip systems belonging to the family. The self-consistent scheme is based on an equivalent inclusion method where each grain is treated as an ellipsoidal inclusion inside the homogeneous equivalent medium (HEM) i.e. the polycrystalline matrix. The
mechanics of the inclusion is solved using a Green’s function approach. Since individual grains interact only with HEM, the overall model is referred to as a one-site model. Each grain comprising a polycrystal has a crystal lattice orientation, an ellipsoidal shape, and a volume fraction. The former two evolve with plastic strain. The matrix has unknown tangent stiffness which is to be determined by enforcing the macroscopic stress and strain rate to be volume averages of the corresponding single crystal quantities:

\[ \dot{\sigma} = \langle \dot{\sigma}^c \rangle; \dot{\epsilon} = \langle \dot{\epsilon}^c \rangle. \] (3)

In Eq. (3), the polycrystal Jaumann stress rate and strain rate are expressed as the volume average of the corresponding grain, \( c \), quantities. These macroscopic quantities are linked using:

\[ \dot{\sigma} = L \dot{\epsilon}, \] (4)

where \( L \) is the unknown instantaneous elasto-plastic stiffness four-rank tensor calculated iteratively using the SC procedure [52, 74]. The Cauchy stress rate is related to the Jaumann stress rate using [75]:

\[ \dot{\sigma} = \dot{\sigma} + \langle W^c \sigma^c \rangle - \langle \sigma^c W^c \rangle = L \dot{\epsilon} + \langle W^c \sigma^c \rangle - \langle \sigma^c W^c \rangle, \] (5)

where \( W^c \) is an elastic spin per grain, \( c \), which will be defined shortly. Equation (5) is integrated over straining time explicitly for obtaining the macroscopic Cauchy stress.

The local strain rate per crystal, \( c \), and the overall strain rate are related using a localization tensor:

\[ \dot{\epsilon}^c = A^c \dot{\epsilon}. \] (6)
The localization tensor for a given instantaneous local elasto-plastic stiffness $\mathbf{L}^c$ is

$$
\mathbf{A}^c = (\mathbf{L}^c + \mathbf{L}^c^*)^{-1}(\mathbf{L}^c^* + \mathbf{L}),
$$

(7)

where, $\mathbf{L}^c^* = \mathbf{L}(\mathbf{S}^c^{-1} - 1)$ is the effective stiffness from the interaction equation: $(\mathbf{\hat{\sigma}}^c - \mathbf{\hat{\sigma}}) = -\mathbf{L}^c^*(\mathbf{\dot{\varepsilon}}^c - \mathbf{\dot{\varepsilon}})$. $\mathbf{S}^c$ is the symmetric portion of the Eshelby tensor while $\mathbf{I}$ is a fourth rank identity. Finally, the above relations result in an implicit equation for macroscopic (matrix) tangent stiffness:

$$
\mathbf{L} = \langle \mathbf{L}^c \mathbf{A}^c \rangle (\mathbf{A}^c)^{-1}.
$$

(8)

At the grain/local level, the constitutive relation is:

$$
\mathbf{\hat{\sigma}}^c = \mathbf{C}^c (\mathbf{\dot{\varepsilon}}^c - \sum_s \mathbf{m}^{c,s}\dot{\gamma}^{c,s}) - \mathbf{\sigma}^c tr(\mathbf{\dot{\varepsilon}}^c),
$$

(9)

where $\mathbf{C}^c$ is the fourth rank elastic stiffness tensor, $\sum_s \mathbf{m}^{c,s}\dot{\gamma}^{c,s}$ is the plastic strain rate made up of slip system shearing rates, $\dot{\gamma}^{c,s}$, and $\mathbf{m}^{c,s} = 0.5(\mathbf{b}^{c,s} \otimes \mathbf{n}^{c,s} + \mathbf{n}^{c,s} \otimes \mathbf{b}^{c,s})$, where $\mathbf{b}^{c,s}$ and $\mathbf{n}^{c,s}$ are the slip system direction and plane normal, respectively.

To activate a slip system $s$, a resolved shear stress on it lowered by backstress, $\tau_{bs}^{c,s}$, must reach its slip resistance, $\tau_c^{c,s}$, i.e. $\mathbf{m}^{c,s} \cdot \mathbf{\sigma}^c - \tau_{bs}^{c,s} = \tau_c^{c,s}$ and the stress has to remain on the evolving crystal yield surface i.e., $\mathbf{m}^{c,s} \cdot \mathbf{\hat{\sigma}}^c - \dot{\tau}_{bs}^{c,s} = \dot{\tau}_c^{c,s}$. The slip resistance defines single crystal yield surface. The addition of the backstress term introduces kinematic hardening effects at a slip system level. Therefore, single crystal yield surface expands with deformation as defined with the slip resistance term, $\tau_c^{c,s}$, and moves as defined with the backstress term, $\tau_{bs}^{c,s}$. Note that there are two slip systems because the two opposite shearing senses are on the same plane.
The slip resistance and backstress evolve with the shearing rates using:

\[
\dot{\tau}_c^{c,s} = \sum_{s'} h^{ss'} h^{c,s'}, \\
\dot{\tau}_b^{c,s} = \sum_{s'} h_{bs}^{ss'} \gamma^{c,s'},
\]

(10)

(11)

where \( h^{ss'} \) and \( h_{bs}^{ss'} \) are the hardening matrix and the backstress matrix, respectively, whose expressions depend on the adopted hardening and backstress evolution laws. The \( h^{ss'} \) and \( h_{bs}^{ss'} \) need to be pre-determined in order to solve the elasto-plastic self-consistent problem. They can either be constant or defined as a function of state variables. For our purpose, we consider \( h^{ss'} \) and \( h_{bs}^{ss'} \) to be functions of accumulated shear strain on slip systems, \( \gamma^s \). The expressions for \( h^{ss'} \) and \( h_{bs}^{ss'} \) are defined in the following sections. Finally, the crystal constitutive law is:

\[
\tilde{\sigma}^c = L^c \dot{\varepsilon}^c,
\]

(12)

where \( L^c \) is:

\[
L^c = C^c - C^c \sum_s m^{c,s} \otimes \left( \sum_{s'} \left( X^{ss'} \right)^{-1} m^{c,s'} (C^c - \sigma^c \otimes i) \right) - \sigma^c \otimes i,
\]

(13)

with:

\[
X^{ss'} = h^{ss'} + h_{bs}^{ss'} + C^c \cdot m^{c,s} \otimes m^{c,s'}.
\]

(14)

Note that indices \( s \) and \( s' \) in Eqs. (13) and (14) go only over active slip systems. Therefore, while full hardening and backstress matrices are used for updating slip resistance and backstress, only a portion of them is used for the calculation of tangent stiffness.
The grain spin tensor necessary for texture evolution, \( W^c \), is:

\[
W^c = W^{app} + \Pi^c - W^{p.c},
\]  

where \( W^{app} \) is the applied spin, \( \Pi^c \) is the spin calculated from an applied macroscopic strain rate to the polycrystal and the antisymmetric part of the Eshelby tensor for grain \( c \) [26], and \( W^{p.c} \) is the plastic spin. The plastic spin is:

\[
W^{p.c} = \sum_s q^{c.s} \gamma^{c.s},
\]  

where \( q^{c.s} = 0.5(b^{c.s} \otimes n^{c.s} - n^{c.s} \otimes b^{c.s}) \).

### 3.1 Dislocation-based hardening law incorporating latent hardening

We use the notation which distinguishes between arbitrarily chosen positive \( s^+ \) and negative \( s^- \) directions of slip systems, while the index \( s \) refers to both directions. Dislocation-based strain rate and temperature sensitive hardening law is used to evolve slip resistance [76-81]. The dislocation-based hardening law was implemented within EPSC first in [82] and used in several other studies [83-85]. The slip resistance is defined as:

\[
\tau^s_c = \tau^s_0 + \tau^s_{\text{forest}} + \tau^s_{\text{debris}},
\]  

where:

\[
\tau^s_{\text{forest}} = b^\alpha \mu^\alpha \sqrt{\sum_s L_{ss'}}^t \rho_{tot}^{s't}
\]  

\[
\tau^s_{\text{debris}} = k_{\text{deb}} \mu^\alpha b^\alpha \sqrt{\rho_{\text{deb}}} \log \left( \frac{1}{b^\alpha \sqrt{\rho_{\text{deb}}}} \right)
\]
where $\tau_0^\alpha$ is an initial slip resistance including: the Peierls stress, solid solution contribution, precipitation contribution, and the Hall-Petch-like effect, $\tau_{forest}^s$ is a forest term arising from statistically stored dislocations, $\tau_{debris}^\alpha$ is a debris term coming from dislocations stored as debris. $b^\alpha = 2.86 \times 10^{-10}$ m is the Burgers vector, $\chi = 0.9$ is an interaction constant, $\rho_{tot}^s$ is the total forest dislocation density for $s^{th}$ slip system ($s \in \alpha$) and $L^{ss'}$ is a latent hardening matrix aka a strength interaction matrix [9, 86]. Magnitude of off-diagonal entries in the strength interaction matrix, $L^{ss'}$, controls the magnitude of the off-diagonal entries in the hardening matrix, $h^{ss'}$. In Eq. (19), $k_{deb} = 0.086$ is a material independent constant and $\rho_{deb}$ is the debris dislocation density [87].

Equation (18) is a modified Taylor relationship for the evolution of slip resistance accounting for dislocation densities on different slip systems and their interactions through the strength interaction matrix. Thus, the evolution of slip resistance depends on the accumulation of immobile dislocations and dislocation interactions. Both increase in dislocation density and dislocation interactions between some slip systems lead to a decrease of the mean free path. Previous study on anisotropy in AA6060 showed that the general trends of anisotropy in flow stress can be captured using latent hardening [9], where several different interaction matrices from the literature have been tested. A stronger latent hardening than the self-hardening is what all these interaction matrices have in common. However, the current EPSC formulation (for convenience, we will refer to this formulation as the standard EPSC) is unable to converge for such strength interaction matrices, due to the loss of ellipticity of the macroscopic tangent modulus. The issue is resolved in the present paper by proposing diagonalization of the hardening matrix, which will be described shortly.
The strength interaction matrix, $L^{ss'}$, has in general 24 x 24 elements, since each slip system within \{111\}(1\overline{1}0) family of 12 slip systems has positive, $s^+$, and negative, $s^-$, direction, which are treated independently. Components of the strength interaction matrix describe different dislocation interactions, which will be described later. The coefficients of the strength interaction matrix can be evaluated experimentally or by use of dislocation dynamics and atomistic simulations [10, 50]. The strength interaction matrix is constant and does not evolve with deformation.

Thus far, slip resistance has been defined in terms of the total forest and debris dislocation densities. Next, an evolution law for dislocation densities in terms of shear strain on slip systems is defined. The evolution of total forest dislocation density during reversed loading takes a different form than the one during forward loading. The origin of altered evolution law during reversal is the annihilation of portion of stored dislocations. The evolution laws for dislocation densities, which take into account annihilation of stored dislocations during load reversal, have been developed in [88, 89]. The dislocation evolution laws from [88] have been implemented into EPSC hardening law in our previous works [53]. The total dislocation density is written as:

$$
\rho_{tot} = \rho_{for}^s + \rho_{rev}^{s^+} + \rho_{rev}^{s^-},
$$

(20)

where $\rho_{for}^s$ is the forward dislocation density and $\rho_{rev}^{s^+}$ and $\rho_{rev}^{s^-}$ are the reversible dislocation densities associated with the $s^+$ and $s^-$ directions, respectively. The three dislocation densities are evolved as functions of shear strain and shearing direction [9, 88, 90]:

(If $d\gamma^{s^+} > 0$)
\[ \frac{\partial \rho^s_{\text{for}}}{\partial y^s} = (1 - p)k_1^\alpha \sqrt{\sum_{st} g^{sst} \rho^s_{\text{tot}}} - k_2^\alpha (\dot{\varepsilon}, T) \rho^s_{\text{for}}, \] (21a)

\[ \frac{\partial \rho^{s+}_{\text{rev}}}{\partial y^s} = p k_1^\alpha \sqrt{\sum_{st} g^{sst} \rho^s_{\text{tot}}} - k_2^\alpha (\dot{\varepsilon}, T) \rho^{s+}_{\text{rev}}, \] (22a)

\[ \frac{\partial \rho^{s-}_{\text{rev}}}{\partial y^s} = -k_1^\alpha \sqrt{\sum_{st} g^{sst} \rho^s_{\text{tot}}} \left( \frac{\rho^{s-}_{\text{rev}}}{\rho_0} \right)^m, \] (23a)

(if \( d\gamma^{-} > 0 \))

\[ \frac{\partial \rho^s_{\text{for}}}{\partial y^s} = (1 - p)k_1^\alpha \sqrt{\sum_{st} g^{sst} \rho^s_{\text{tot}}} - k_2^\alpha (\dot{\varepsilon}, T) \rho^s_{\text{for}}, \] (21b)

\[ \frac{\partial \rho^{s+}_{\text{rev}}}{\partial y^s} = -k_1^\alpha \sqrt{\sum_{st} g^{sst} \rho^s_{\text{tot}}} \left( \frac{\rho^{s+}_{\text{rev}}}{\rho_0} \right)^m, \] (22b)

\[ \frac{\partial \rho^{s-}_{\text{rev}}}{\partial y^s} = p k_1^\alpha \sqrt{\sum_{st} g^{sst} \rho^s_{\text{tot}}} - k_2^\alpha (\dot{\varepsilon}, T) \rho^{s-}_{\text{rev}}, \] (23b)

with the following initial conditions:

\[ \rho^{s}_{\text{for}}(\gamma^s = 0) = 10^{11} \text{ m}^{-2}, \rho^{s+}_{\text{rev}}(\gamma^s = 0) = 0 \text{ and } \rho^{s-}_{\text{rev}}(\gamma^s = 0) = 0, \] (24)

where \( k_1^\alpha \) is a coefficient controlling the rate of generation of statistically stored dislocations, \( k_2^\alpha \) is a rate-sensitive coefficient for dynamic recovery [78], \( p \) is a reversibility parameter having a value between 0 and 1, and \( g^{sst} \) is another interaction matrix, which defines the strength of dislocation interaction governing solely the accumulation of forest dislocations on slip system \( s \) depending on the dislocation density on system \( s' \). Analogy between \( L^{sst} \) for slip resistance to \( g^{sst} \) for the rate of dislocation evolution is evident. The interaction matrix for dislocation storage is a constant matrix and is inspired by the previous works [9, 91, 92]. The \( g^{sst} \) is a constant
matrix not expected to evolve with deformation. The effect of entries of $g^{ss'}$ matrix on mechanical response is discussed in results section. Note that $g^{ss'}$ does not create off-diagonal terms in hardening matrix, $h^{ss'}$. The reversibility parameter controls the fraction of total dislocation density that evolves as reversible dislocation density. In Eqs. (22b) and (23a), $m$ is a parameter accounting for the rate of dislocation recombination having value of 0.5 [93] and $\rho_0^s$ is the total dislocation density at the moment of shear reversal on the $s^{th}$ slip system [94].

The rate-sensitive coefficient for dynamic recovery, $k_2^s$, is:

$$\frac{k_2^s}{k_1^s} = \frac{e^{b\alpha}}{g^\alpha} \left( 1 - \frac{k_B T}{D^\alpha (b\alpha)^3} \ln \left( \frac{\dot{\epsilon}}{\dot{\epsilon}_0} \right) \right),$$

(25)

where, $k_B$, $\dot{\epsilon}_0$, $g^\alpha$ and $D^\alpha$ are the Boltzmann constant, a reference strain rate taken to be $10^7$ s$^{-1}$, an effective activation enthalpy and a drag stress, respectively. The evolution law for debris dislocation density is:

$$\frac{\partial \rho_{deb}^d}{\partial y^D} = q^\alpha b^\alpha \sqrt{\rho_{deb}} k_2^s(\dot{\epsilon}, T) \rho_{tot}^s,$$

(26)

where $q^\alpha$ is a dislocation recovery rate constant that extracts a fraction of $\alpha$-type dislocations that do not annihilate but become debris from those that do annihilate. Initial content of debris dislocation density is taken to be $0.1 \ m^{-2}$.

### 3.2 Backstress evolution law

To also aid in capturing the effect of strain path reversal, the slip system backstress evolution is considered, using an empirical law. The implementation of a backstress law in EPSC was first presented in [73]. Here we consider an evolution law
for backstress per slip system based on the work presented in [54, 95]. In the empirical formulation employed here, we first define slip system sources of backstress which evolve with shear strain. All sources of backstresses on individual slip systems are superimposed to form the backstress tensor as proposed in [96]. The backstress tensor is then projected on individual slip systems to arrive to the final expression of backstress. The final expression for backstress on a slip system, $\tau_{bs}^s$, is:

$$\tau_{bs}^s = \mathbf{m}^s \cdot \sigma_{bs}^c = \tau_{bs,sys}^s + 2 \sum_{s'} \mathbf{m}^s \cdot \mathbf{m}^{s'} \tau_{bs,sys}^{s'},$$

(27)

with

$$\tau_{bs,sys}^{s'} = \begin{cases} \tau_{bs,sys}^{s'} & \text{if } \tau_{bs,sys}^{s'} > 0 \\ 0 & \text{if } \tau_{bs,sys}^{s'} < 0 \end{cases}$$

(28)

where $\sigma_{bs}^c$ is backstress tensor formed by superimposing slip system sources of backstress, $\tau_{bs,sys}^{s'}$, and the sum over $s'$ spans over all slip systems and $s' \neq s$. We adopt following functions for the evolution of $\tau_{bs,sys}^s$ with shear strain:

$$\text{if } d\dot{\gamma}^s > 0 \text{ and } \tau_{bs,sys}^{s+} > 0$$,

$$\tau_{bs,sys}^{s+} = \tau_{bs}^{sat} (1 - \exp(-\nu \gamma^{s+})),$$

(29)

$$\tau_{bs,sys}^{s-} = -A \tau_{bs,sys}^{s+},$$

(30)

$$\text{if } d\dot{\gamma}^s > 0 \text{ and } \tau_{bs,sys}^{s+} < 0$$,

$$\tau_{bs,sys}^{s+} = -(A + 1) \tau_{bs}^{sat} \exp\left(-\frac{\gamma^{s-}}{\gamma_b}\right) + \tau_{bs}^{sat},$$

(31)
\[
\tau_{bs,sys}^s = -\frac{1}{A}\tau_{bs,sys}^s
\]  
(32)

where \( \tau_{bs}^{sat} \) is a saturation value for backstresses, A is a parameter for asymmetric evolution of backstress on a slip system in two different directions \( s^+ \) and \( s^- \), \( \gamma_b \) and \( \nu \) are material parameters. The shear strain \( \gamma^s \) is recorded from the point of local load reversal.

### 3.3 Analytical description of the hardening matrix, \( h^{ss'} \), and the backstress matrix, \( h_{bs}^{ss'} \)

To complete the set of relations pertaining to the EPSC formulation, the hardening matrix \( h^{ss'} \), and the backstress matrix, \( h_{bs}^{ss'} \), remain to be defined. Following Eqs. (10) and (11), entries of these matrices are partial derivatives:

\[
h^{ss'} = \frac{\partial \tau_c^s}{\partial \gamma^{s'}}; \quad h_{bs}^{ss'} = \frac{\partial \tau_{bs}^s}{\partial \gamma^{s'}}.
\]  
(33)

Therefore, in order to define the hardening matrix, \( h^{ss'} \), a function \( \tau_c^s = \tau_c^s(\gamma^{s'}) \) defining the evolution of slip resistance with shear strain on slip systems needs to be available. Similarly, to define the backstress matrix, \( h_{bs}^{ss'} \), an evolution function \( \tau_{bs}^s = \tau_{bs}^s(\gamma^{s'}) \) needs to be available. The expressions for \( h^{ss'} \) and \( h_{bs}^{ss'} \) are provided in appendix A for the evolution laws used in the present study.

### 3.4 Solution procedure for single crystal stress increment after introducing effects of latent hardening

The latent hardening is introduced in the model through the use of the strength interaction matrix, \( L^{ss'} \), in Eq (18). The strength interaction matrix affects the hardening matrix, \( h^{ss'} \) (appendix A). More specifically, it affects the ratio between elements on the
diagonal to the off-diagonal elements in $h^{ss'}$ for active slip systems. The positive definiteness of the hardening matrix is a necessary condition for the determination of shear rates on active slip system in rate independent formulation [97]. However, the positive definiteness of $h^{ss'}$ is not expected when latent hardening is stronger than self-hardening, since the largest elements of the matrix are not on the diagonal [98].

The realistic (experimentally measured) latent hardening constants as presented in the literature for Al and Al alloys [9, 10, 13] result in larger latent hardening than self-hardening. As a result, computational issues arise both at single crystal and polycrystalline levels. In this section, the single crystal issues are treated, while in the next section we treat issues at polycrystal level.

The single crystal solution procedure involves the determination of a set of active slip systems and shear increments on active slip systems given an imposed single crystal increment in strain. The procedure begins by determining a set of potentially active slip systems fulfilling the loading condition $m^s \cdot \sigma^c - \tau_{bs}^s = \tau_c^s$. Next, shear increments are determined for all potentially active slip systems by enforcing the consistency condition, $m^s \cdot \dot{\sigma}^c - \dot{\tau}_{bs}^s = \dot{\tau}_c^s$, producing the system of linear equations:

$$\Sigma_{s'}(h^{ss'} + h_{bs}s' + C^c \cdot m^s \otimes m^{s'}) \Delta \gamma^{s'} = m^s (C^c - \sigma^c \otimes i) \Delta \varepsilon^c.$$  \hspace{1cm} (34)

Evidently, the matrix, $X^{ss'}$, defined in Eq. (14) needs to be inverted in order to solve for shear increments, $\Delta \gamma^{s'}$, on potentially active slip systems. If any of the resulting shear increments is negative, then that slip system is removed from the set of potentially active slip systems and shear increments are recalculated. Slip systems are eliminated
from the initial set of potentially active slip systems until all active slip systems have positive shear increments. In addition, inactive slip systems must satisfy \( \mathbf{m}^s \cdot \mathbf{c}^c - \tau_{bs}^s \leq \tau_c^s \), i.e. stress cannot get out of the single crystal yield surface. The final set of active slip systems is used in calculating the tangent stiffness of single crystals (Eq. 13).

Two possible issues can arise in the above presented procedure. The first issue is singularity of the matrix \( X^{ss'} \). The problem has been treated in literature [16, 99-102]. We adopt the approach of [16], where a singular value decomposition procedure of \( X^{ss'} \) is proposed:

\[
X = U W V^T
\]

(35)

where \( U \) and \( V \) are orthogonal matrices, while \( W \) is a diagonal matrix with singular values of \( X \) positioned along the diagonal. The pseudo inverse of matrix \( X^+ \) is then:

\[
X^+ = V W^+ U^T
\]

(36)

where \( W^+ \) is diagonal matrix given with:

\[
W^{ss} = \begin{cases} 
1/W^{ss} & \text{if } W^{ss} / \max W^{ss} > 1e - 12 \\
0 & \text{if } W^{ss} / \max W^{ss} < 1e - 12 
\end{cases}
\]

(37)

The second issue that rarely occurs is inability to find a set of active slip systems satisfying all constraints for an arbitrary hardening law. We observe that in some cases the elimination of slip systems with negative shear increments violates the condition \( \mathbf{m}^s \cdot \mathbf{c}^c - \tau_{bs}^s \leq \tau_c^s \) for some of the eliminated slip systems at the end of the applied increment. A couple of percent of all active slip systems can exhibit this problem with introduction of latent hardening more pronounced than self-hardening. The percent of
slip systems where stress exits the single crystal yield surface is dependent on adopted interaction matrix for dislocation density evolution, \( g^{ss'} \), and strength interaction matrix, \( L^{ss'} \). If stress exits the yield surface on some slip systems, the slip resistance is corrected so that stress remains on the single crystal yield surface i.e. slip resistance is enforced to be \( \tau^s_c = \mathbf{m}^s \cdot \mathbf{\alpha}^c - \tau^s_{bs} \).

**3.5 Singularity in the Eshelby tensor calculation upon introducing effects of latent hardening**

Using the methods presented in the previous section, solution to single crystals can be found for a given hardening law. However, issues are also encountered within the homogenization procedure, i.e. in the Eshelby tensor calculation.

The general symmetric Eshelby tensor, defining the strain rate inside the inclusion, can be calculated in terms of the Green’s function [103]. The Green’s function in Fourier space is calculated using:

\[
k^2 \hat{G}_{in} = (\alpha_i \alpha_j L_{i j n l})^{-1}, \tag{38}
\]

where \( \hat{G}_{in} \) is the Green’s function in Fourier space and \( \mathbf{k} \) is a point vector of the Fourier space with magnitude \( k \) and in direction of a unit vector \( \mathbf{\alpha} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta) \) (i.e. \( \mathbf{k} = k\mathbf{\alpha} \)).

The possible issue in the Eshelby tensor calculation is singularity of the 2\(^{nd}\) rank tensor \( \alpha_i \alpha_j L_{i j n l} \) for certain values of the angles \( \theta \) and \( \varphi \), over which integration is performed to define the Eshelby tensor in real space. This condition can be expressed as:
\[
\det(\alpha_i \alpha_j L_{ijn}) = 0,
\]

which is referred to as the loss of ellipticity of the tangent stiffness and can be related to bifurcation and/or shear band formation [104]. In contrast, the strong ellipticity of tangent stiffness is desirable and defined as:

\[
L_{ijn} x_i y_j x_n y_l = (L_{ijn} y_j y_l) x_i x_n = Q_{in} x_i x_n > 0,
\]

where \(Q_{in}\) is the acoustic tensor [105] and \(x_i\) and \(y_j\) are arbitrary unit vectors. For \(L_{ijn}\) to be strongly elliptical, the acoustic tensor needs to be positive definite, which implies that \(\det Q_{in} \neq 0\) [105]. The strong ellipticity of the tangent stiffness is a necessary condition for solvability of the equivalent inclusion problem for an ellipsoidal inhomogeneity [106]. If the differential equations of equilibrium are elliptic, the condition of strong ellipticity is satisfied.

We notice that tangent stiffness loses ellipticity when the latent hardening is more pronounced than the self-hardening. This implies that the use of the theory 1 of latent hardening leads to loss of ellipticity, while the use of the theory 2 of latent hardening does not cause the loss of ellipticity because the matrix is diagonal. The same effect of the theory 1 latent hardening on the loss of ellipticity of governing equations for single crystals was noted in [15]. Similar issues are encountered in the case of simulating softening in materials [107]. Problems with the loss of ellipticity can be avoided by introducing the rate-dependence i.e. visco-plasticity [108, 109]. Introducing strain rate sensitivity in the rate-independent framework of EPSC is left for future developments.
The loss of strong ellipticity condition for overall tangent stiffness of a polycrystal appears to be related to the loss of ellipticity of single crystals tangent stiffness tensors constituting the polycrystal. Therefore, before investigating the overall tangent stiffness tensor, we investigate the behavior of tangent stiffness tensors of single crystals in function of the ratio between diagonal and off-diagonal terms in their respective hardening matrices.

A crystal with Bunge-Euler angles (23, 12, 308) is arbitrarily chosen for the analysis. Four slip systems with the highest Schmid factor under tension along the direction 1 are assumed to be active in constructing the tangent stiffness, \( \mathbf{L}^c \), according to Eqs. (13) and (14). The hardening matrix to facilitate the analysis is arbitrarily set to give a reasonable hardening rate as follows:

\[
    k^{ss'} = \begin{cases} 
        1000 & \text{if } s = s' \\
        h_r 1000 & \text{if } s \neq s'
    \end{cases},
\]

where \( h_r \) defines the off-diagonal entries and \( s \) and \( s' \) go over active the slip systems. The single crystal stress in Eq. (13) is assumed to be zero, while the single crystal elastic stiffness, \( \mathbf{C}^c \), is based on the single crystal elastic constants for Al \([110]\). We calculate the acoustic tensor of the single crystal tangent stiffness and its maximum condition number \( (c_{\text{max}}) \). By definition, the condition number is the ratio between the largest and the smallest singular value of a matrix \([111]\). To achieve the maximum of the ratio, the vectors \( y_j \) and \( y_l \) in Eq. (40) are varied using the function ‘fminunc’ in Matlab to perform unconstrained optimization. Figure 6 shows a plot of the condition number vs. \( h_r \). Evidently, the acoustic tensor becomes near singular for \( h_r > 1 \). A similar conclusion for the behavior of single crystals was presented in [15].
Next, we sample 200 crystals from the ODF shown in Fig. 2c and apply the hardening law given by Eq. (41). We set $h_r$ to 1.5, the initial value of slip resistance to 50 MPa, and simulate simple tension of the polycrystal using EPSC. Figure 4 shows the simulation results. The true stress-true strain curve (Fig. 4a) is plotted up to the strain level at which the EPSC is no longer able to solve for homogenized tangent stiffness. The fraction of grains having the max condition number of acoustic tensor greater than $1 \times 10^8$ is shown in Fig. 4b indicating that the number of grains losing ellipticity is increasing with strain. Our analysis shows that the macroscopic tangent stiffness has nearly lost ellipticity and therefore, the solution procedure in EPSC is breaking down. With further straining more grains would lose ellipticity and the overall tangent stiffness would lose ellipticity when nearly all grains lose their ellipticity [104].

From the above presented analysis, we conclude that the theory 1 description of latent hardening with experimentally evaluated latent hardening coefficients leads to the loss of ellipticity of the overall tangent stiffness.

![Fig. 3. Maximum condition number of acoustic tensor as a function of the ratio between diagonal and off-diagonal terms in the hardening matrix.](image-url)
3.6 Overcoming the loss of ellipticity

This section presents two methods used to suppress the loss of ellipticity, one proposed here and another available from the literature originally proposed to resolve the issue of non-uniqueness in the choice of active slip systems. The methods are based on opposing concepts in terms of the dependence of slip systems, as will become clear from the description below. Both methods have been compared against the latent hardening in the standard EPSC formulation for a case study in which the standard formulation converges. Results of the comparison suggest that the novel method proposed here is well suited for predicting the effect of latent hardening on plastic anisotropy of AA6022-T4.

3.6.1 Diagonalization of the hardening matrix procedure

In order to perform the homogenization procedure, the single crystal tangent stiffness needs to be elliptical. The ellipticity of tangent stiffness of single crystal is a
function of relative size of diagonal and off-diagonal elements of the hardening matrix, as shown in Fig. 3. As stated earlier, the hardening matrix must be a positive definite. To resolve the problem we propose a replacement of the hardening matrix that enters the single crystal tangent stiffness calculation with a hardening matrix that is guaranteed to be positive definite. This matrix is referred to as the diagonalized hardening matrix.

Note that while the single crystal solution procedure involving a given hardening matrix remains as described in section 3.4, the diagonalized hardening matrix is inserted in Eqs. (14) and (13) for the calculation of single crystal tangent stiffness, $L^c$.

The definition of new hardening matrix comes from assuming that both hardening matrices relate to the same hardening law, meaning that increments in slip resistance produced by both matrices should be the same:

$$\sum_{s'} h_r^{ss'} \Delta \gamma^{s'} = \sum_{s'} h^{ss'} \Delta \gamma^{s'}$$  \hspace{1cm} (42)

where $h_r^{ss'}$ is the diagonalized hardening matrix. The indices $s$ and $s'$ in equation (42) go over active slip systems. The diagonalized matrix is written as:

$$h_r^{ss'} = h_d^{ss'} + r h_{off}^{ss'},$$  \hspace{1cm} (43)

where $h_d^{ss'}$ is the unknown matrix with off-diagonal elements equal to zero, $h_{off}^{ss'}$ is a matrix formed from $h^{ss'}$ by setting the matrix entries along the diagonal to zero and $r$ is a diagonalization parameter set to a value between 0 and 1. The indices $s$ and $s'$ in equation (43) go over all slip systems. Replacing equation (43) in (42) allows determination of unknown elements along the diagonal of matrix $h_d^{ss'}$.
\[
 h_d^{ss} \Delta \gamma^s + \sum_{s'} r h_{off}^{ss'} \Delta \gamma^{s'} = \sum_{s'} h^{ss'} \Delta \gamma^{s'} \rightarrow h_d^{ss} = \frac{1}{\Delta \gamma^s} \left( \sum_{s'} h^{ss'} \Delta \gamma^{s'} - r \sum_{s'} h_{off}^{ss'} \Delta \gamma^{s'} \right) .
\]

(44)

where indices \( s \) and \( s' \) go over active slip systems. The diagonalization parameter, \( r \), defines weight of the diagonal elements compared to off-diagonal elements. For instance, when \( r = 0 \) the matrix \( h_{r}^{ss'} \) becomes \( h^{ss'} \) i.e. off-diagonal elements are dominant, while when \( r = 1 \) the matrix \( h_{r}^{ss'} \) becomes \( h_d^{ss'} \) i.e. the matrix is diagonal.

Reducing hardening matrix to its diagonal form can be interpreted as "breaking the dependence" between slip systems in terms of slip resistance. The dependence of slip resistance is introduced by the concept of latent hardening theory \( 1 \), where slip resistance is dependent on shear on all slip systems and the hardening matrix is full.

While the proposed approach does not change the single crystal response, it affects the overall homogenized tangent stiffness. Therefore, the polycrystal response can be slightly altered. To evaluate the effect, we compare the results from this procedure with the results based on the regularized Schmid law \( [112] \). The latter approach is summarized next.

3.6.2 Regularized Schmid law procedure

The regularized Schmid law for the rate-independent crystal plasticity was proposed in \([112]\). The formulation allows predictions of forming limit diagrams using the bifurcation analysis as presented in \([113]\). Here we closely follow derivations from \([114]\), while enforcing the normal to yield surface to have a norm of unity \([115]\). The rotation of
single crystals is neglected for simplicity when deriving the equations and performing the integration. The single crystal yield function is:

\[
f = \left( \sum_s \left( \frac{\sigma^c \cdot m^s}{\tau_c^s + \tau_{bs}^s} \right)^{2N} \right)^{\frac{1}{2N}} - 1 \leq 0,
\]  

(45)

where \( N \) is an integer parameter controlling the radius of single crystal yield surface corners. With known yield function, the normal to yield surface is:

\[
\hat{n} = \left\| \frac{\partial f(\sigma^c)}{\partial \sigma^c} \right\|^{-1} \frac{\partial f(\sigma^c)}{\partial \sigma^c} = \frac{1}{\left\| \sum_s \left( \frac{\sigma^c \cdot m^s}{\tau_c^s + \tau_{bs}^s} \right)^{2N-1} \frac{1}{\tau_c^s + \tau_{bs}^s} m^s \right\|} \sum_s \left( \frac{\sigma^c m^s}{\tau_c^s + \tau_{bs}^s} \right)^{2N-1} \frac{1}{\tau_c^s + \tau_{bs}^s} m^s.
\]  

(46)

The plastic strain rate is:

\[
\dot{\varepsilon}^{pl} = \dot{\Lambda} \hat{n},
\]  

(47)

where \( \dot{\Lambda} \) is the plastic multiplier. Using the expression for plastic strain rate in terms of shear rates, \( \dot{\varepsilon}^{pl} = \sum_s \dot{\gamma}^s m^s \), together with Eqs. (46) and (47) we can express the shear rate as:

\[
\dot{\gamma}^s = \dot{\Lambda} \hat{n}^s,
\]  

(48)

where:

\[
\hat{n}^s = \left\| \sum_s \left( \frac{\sigma^c \cdot m^s}{\tau_c^s + \tau_{bs}^s} \right)^{2N-1} \frac{1}{\tau_c^s + \tau_{bs}^s} m^s \right\| \left( \frac{\sigma^c \cdot m^s}{\tau_c^s + \tau_{bs}^s} \right)^{2N-1} \frac{1}{\tau_c^s + \tau_{bs}^s}.
\]  

(49)

The semi-implicit integration procedure is applied to define the constitutive relation [116]. Details of the integration procedure are given in appendix B. The linearized form of single crystal constitutive law consistent with the integration procedure is:
\[ \Delta \sigma^c = \frac{\partial \Delta \sigma^c}{\partial \Delta \varepsilon^c} \Delta \varepsilon^c + \Delta \sigma^{c,*} = \frac{\partial \Delta \sigma^c}{\partial \Delta \varepsilon^c} (\Delta \varepsilon^c - \Delta \varepsilon^{c,*}) \]  

(50)

where \( \Delta \varepsilon^{c,*} \) is calculated by replacing \( \Delta \sigma^c = C^c(\Delta \varepsilon^c - \Delta \lambda \hat{n}) \) in Eq. (50):

\[ \Delta \varepsilon^{c,*} = \Delta \varepsilon^c - \frac{\partial \Delta \sigma^c}{\partial \Delta \varepsilon^c}^{-1} C^c (\Delta \varepsilon^c - \Delta \lambda \hat{n}). \]  

(51)

The homogenization procedure for the linearized response of non-linear constituents is known as the affine formulation with step-wise reference to a linear comparison medium with an eigenstrain, for each grain and for the overall behavior [117]. The details are presented in appendix C.

The idea behind regularized Schmid law is the introduction of the dependence between slip systems, controlled with the exponent \( N \). Therefore, all slip systems are always active and shear rates between slip systems are connected i.e. shear rate and appearance of slip depends on shear stress on all slip systems. The introduced concept is different from the standard Schmid law which assumes independence between slip systems. In this sense the idea of regularized Schmid law is opposite to the one of diagonalization procedure i.e. regularized Schmid law introduces the dependence between slip systems, while diagonalization procedure is removing the dependence between slip systems.

To validate the single crystal integration procedure, a number of strain increments (\( \Delta \varepsilon_{11} = 1e - 5, \Delta \varepsilon_{22} = -0.5e - 5, \Delta \varepsilon_{33} = -0.5e - 5, \Delta \varepsilon_{12} = \Delta \varepsilon_{13} = \Delta \varepsilon_{23} = 0 \)) are applied to an arbitrary crystal of the following crystal orientation (23,12,308). It is worth mentioning that the amount of strain per increment needs to be sufficiently small to avoid any numerical issues, since the semi-implicit algorithm is employed and the
equations can be very stiff if $N$ is large [118]. The initial slip resistance is set to 50 MPa and the hardening is defined using Eq. (41) with $h_r = 0$. Figure 5 compares predictions from the regularized Schmid law and the usual Schmid law. Evidently, the predictions are identical, validating the implementation of the regularized Schmid law procedure. In addition, the regularized Schmid law predictions with both $N=50$ and $N=100$ give similar results. Increasing the exponent $N$ improves the accuracy at the yield surface corners but also increases the computational time.

![Figure 5](image)

Fig. 5. Comparison of mechanical response for a single crystal deformed by imposing strain increments ($\Delta \varepsilon_{11} = 1e^{-5}$, $\Delta \varepsilon_{22} = -0.5e^{-5}$, $\Delta \varepsilon_{33} = -0.5e^{-5}$, $\Delta \varepsilon_{12} = \Delta \varepsilon_{13} = \Delta \varepsilon_{23} = 0$) for Schmid law and the regularized Schmid law. Two different values of the power-law parameters $N$ are used, which controls the sharpness of the corners of single crystal yield surfaces.

3.6.3 A case study comparing the procedures for overcoming the singularity in the Eshelby tensor calculation: Simple tension of AA6022-T4

In this section, a comparison is made between the standard EPSC and two approaches for overcoming the numerical loss of ellipticity: (1) diagonalization of the hardening matrix procedure and (2) regularized Schmid law procedure. The goals are to quantify their deviation from the standard EPSC by comparing predicted mechanical
responses and to choose a more suitable method for predicting the anisotropy of AA6022-T4. The comparison is performed on the same set of 200 grains sampled from the ODF in Fig. 2c. For simplicity, texture evolution is turned off for the simulations presented in this section, while texture evolution is enabled in all other simulations presented in the following sections. The constant hardening matrix used for theory 2 formulation is:

\[
h^{ss'} = \begin{cases} 
    h_c & \text{if } s = s' \\
    0.95 \times h_c & \text{if } s \neq s'
\end{cases}
\]  

(52)

where \( h_c = 150 \text{ MPa} \) is the chosen hardening rate. Simple tension along the RD is simulated. The same simulation is also performed while using the diagonalization of the hardening matrix and the regularized Schmid law procedures. Since these schemes alter the mechanical response for a given hardening matrix, Eq. (52), the constant hardening rate, \( h_c \), was adjusted such that the three simulations provide approximately the same true stress-true strain response in tension: 126 MPa when \( r = 0 \), 141.5 MPa when \( r = 0.95 \), and 122 MPa for the regularized Schmid law simulations. We remind that for \( r = 1 \), the standard EPSC formulation is retrieved. The initial slip resistance was kept at 50 MPa for simulations with the diagonalization of hardening matrix and standard EPSC, while it was set to 47 MPa for the simulation with the regularized Schmid law. Figure 6a shows the comparison of simulation results, indicating that the mechanical response of all simulations is essentially identical. Figure 6b shows that the predictions of \( r \)-ratio are also similar for all simulations. Figures 6c, d, and e show the deviation of microscopic from macroscopic quantities. The compared quantities are tangent stiffness, strain, and stress rates. In the first case, the difference between single
crystal tangent stiffness tensors and the overall macroscopic stiffness is calculated for
each crystal using \( d^c(L, L^c) = \frac{2||L-L^c||}{||L+L^c||} \) and the volume average is then calculated. It can
be seen that methods for overcoming the loss of ellipticity result in a lower mean
deviation relative to the standard EPSC, meaning that single crystal tangent stiffness
tensors are more similar among different crystal orientations. The deviation of single
crystal strain rate and stress rate is calculated using \( \frac{\sqrt{\langle \left( \ddot{\mathbf{e}} - \ddot{\mathbf{e}}^c \right)^2 \rangle}}{||\ddot{\mathbf{e}}||} \) and \( \frac{\sqrt{\langle \left( \ddot{\mathbf{\sigma}} - \ddot{\mathbf{\sigma}}^c \right)^2 \rangle}}{||\dot{\mathbf{\sigma}}||} \) and
plotted in Figs. 6d and e, respectively, after performing volume averaging. The plot
shows that single crystal strain rate varies less from the macroscopic strain rate for the
methods introduced to overcome the loss of ellipticity than that for the standard EPSC.
However, the regularized Schmid law predicts the most similar strain rates amongst
grains, resembling the Taylor iso-strain homogenization assumption, which was also
noted in [114]. The stress rate deviation behaves in the opposite manner to strain rate
deviation. As expected, the diagonalization of hardening matrix with the diagonalization
parameter of \( r = 0.95 \) predicts the response which is the closest to the standard EPSC.

From the analysis presented in this section we conclude that the diagonalization
of hardening matrix gives results more similar to the standard EPSC than the
regularization of Schmid law. The regularized Schmid law procedure served as a
reference for comparing the developed hardening matrix diagonalization procedure, but
in itself is very computationally involved, especially for \( N>50 \), since it has the semi-
implicit integration algorithm. The new procedure developed herein for overcoming the
loss of ellipticity enabled the use of experimentally determined latent hardening
Fig. 6. Comparison of: (a) true stress-true strain curves, (b) r-ratio, (c) volume average of the difference between single crystal and macroscopic tangent stiffness, (d) the volume average difference between single crystal strain rate and applied strain rate and (e) the volume average difference between single crystal stress rate and applied stress rate, calculated by models indicated in the legend.
constants. It should be noted that the diagonalization of hardening with $r=0$ matrix procedure gives diagonal hardening matrix for active slip systems, conforming to theory 2 latent hardening [14, 17, 18]. The developed procedure with EPSC is used in the subsequent sections for predicting the anisotropy of AA6022-T4 alloy.

4. Results and discussion

4.1 Predictions using the standard EPSC model

We begin by presenting the predictions using the model without the modifications pertaining to the hardening [53]. Hardening along with latent hardening and backstress parameters are calibrated towards the data in Fig. 2. We emphasize that the crystallographic texture is mainly governing the anisotropy in this case.

The simple tension simulations are performed by enforcing increments in strain in a given direction of tension, while keeping the lateral stresses and shear strains at zero. The three measured stress-strain curves were used for fitting the hardening law parameters, while simulation results for $r$-ratio are considered as predictions. Table 1 shows the best fit parameters established for AA6022-T4. Theory 1 of latent hardening was used with the self-hardening coefficients set to unity ($L_{ss} = 1$) and the latent hardening coefficients set to 0.99 ($L_{ss'} = 0.99$ with $s \neq s'$), since the magnitude for the latter coefficients of 1 or greater causes loss of ellipticity for single crystals. As discussed, the use of more realistic (experimentally established) latent hardening coefficients is not possible within the standard EPSC implementation due to convergence issues. The starting measured texture shown in Fig. 2b was used to generate an input orientation distribution function (ODF) with MTEX matlab tool box [119], where 2000 weighted orientations were appropriately sampled and used as the
starting texture for simulations. The invariant single crystal elastic constants for Al are: $C_{11} = 108.2$ GPa, $C_{12} = 61.3$ GPa, and $C_{44} = 28.5$ GPa [120].

Fig. 7. Comparison of predictions using the standard EPSC and measurements for AA6022-T4: (a) true stress-true strain response and (b) r-ratio.

Figure 7 shows the predictions in terms of true stress-true strain response and r-ratio. Evidently, the anisotropy in the mechanical response is not well predicted. Note that lateral strain components (those in 22 and 33 directions if the loading is in 11 direction), which determine the r-ratio, are calculated from a system of linear equations given with Eq. (12). The system is solved using known values of strain rate and Jaumann stress rate, which are based on imposed boundary conditions. The solution for the system of linear equations in terms of the unknown strain rates in the directions 22 and 33 is in function of $L_{21}, L_{22}, L_{23}, L_{31}, L_{32}$ and $L_{33}$ components of the polycrystal tangent stiffness tensor of HEM. The homogenous effective medium is a fictitious homogenous material that behaves in the same way as the heterogeneous polycrystal. The tangent stiffness of the HEM is dependent on the selected homogenization
approach, single crystal tangent stiffness, and texture. The single crystal tangent stiffness depends on the adopted hardening law. Therefore, the hardening law integrating the latent hardening and texture evolution govern the r-ratio evolution within the self-consistent homogenization approach used here. Thus, in our model, the predicted r-ratio is a direct consequence of the evolution of the polycrystal tangent stiffness, originating in the hardening rate and texture.

Table 1a. Constitutive parameters for the evolution of slip resistance for \{111\}(1\overline{1}0) slip mode in AA6022-T4.

<table>
<thead>
<tr>
<th>$\tau_0$ [MPa]</th>
<th>$k$ [$m^{-1}$]</th>
<th>$g$</th>
<th>$D$ [MPa]</th>
<th>$q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td>1.4 x10</td>
<td>0.0784</td>
<td>100</td>
<td>16</td>
</tr>
</tbody>
</table>

Table 1b. Parameters for the evolution of slip system kinematic backstress in AA6022-T4.

<table>
<thead>
<tr>
<th>$\tau_{\text{bs}}^{\text{sat}}$ [MPa]</th>
<th>$\nu$</th>
<th>$\gamma_b$</th>
<th>$A$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>560</td>
<td>0.001</td>
<td>10</td>
</tr>
</tbody>
</table>

Next, we present results in terms of predicted plastic anisotropy of AA6022-T4 using EPSC formulation with the diagonalization of the hardening matrix procedure and the singular value decomposition along with the penalty stiffness procedure for solving for single crystal stress increment. Predictions of mechanical response will allow us to discuss the origin of plastic anisotropy in the material.

4.2 Predictions based on the strength interaction matrix, $L^{ss'}$

The strength interaction matrix in Eq. (18) is defined to contain six independent coefficients aimed at describing six types of dislocation interactions. The possible dislocation interactions are: (1) self-interaction between dislocations belonging to the same slip system, (2) coplanar-interaction between dislocations on the same slip plane,
(3) interaction resulting in Hirth lock, (4) collinear interaction between dislocations on cross slip planes, (5) interaction resulting in sessile Lomer-Cottrell locks, and (6) glissile lock. However, a recent study involving latent hardening models utilizing up to six interaction coefficients revealed that the simplified strength interaction matrix of two entries were sufficiently general to predict anisotropy in FCC metals [9]. Here, we assumed the self-hardening and the coplanar interactions as unity, while the other interactions were set to 1.4 consistent with the measurements performed on Al single crystals in [13]. Thus, the interaction matrix is reduced to two independent coefficients, governing the self and latent hardening. Several earlier studies made the same assumption [15, 16, 121]. The fitted hardening law parameters are given in Table 2. The interaction matrix used in the evolution law for dislocation density (Eqs. 21-23) is $g^{ss} = 1$ and $g^{ss'} = 0$ with $s \neq s'$. The fitted parameters for backstress are given in Table 1b.

![Fig. 8. Comparison of the predictions and measurements for AA6022-T4: (a) true stress-true strain response and (b) r-ratio.](image_url)
The results are shown in Fig. 8. The simulated stress-strain curves to larger plastic strains follow the same trend as measured curves. However, the 45 direction stress is slightly over-predicted, while the TD direction stress is slightly under-predicted. The predictions of r-ratio follow similar trends as measurements, while the actual values are not matching very well needing further investigation. We note that the r-ratio predictions are not affected by the strength interaction matrices and that with the diagonalization of hardening matrix procedure, we no longer observe the decreasing r-ratio with plastic strain.

Table 2. Constitutive parameters for the evolution of slip resistance for \(\{111\}\langle 1\bar{1}0\rangle\) slip mode in AA6022-T4.

<table>
<thead>
<tr>
<th>(\tau_0) [MPa]</th>
<th>(k_1) ([m^{-1}])</th>
<th>(g)</th>
<th>(D) [MPa]</th>
<th>(q)</th>
</tr>
</thead>
<tbody>
<tr>
<td>56</td>
<td>1.3 (\times 10^8)</td>
<td>0.0618</td>
<td>100</td>
<td>8</td>
</tr>
</tbody>
</table>

To highlight the effect of latent hardening on plastic anisotropy in the flow curves of AA6022-T4, several simulations were run with the self-hardening \(L^{ss'}\) set to 1.0, while the latent hardening \(L^{ss'}\) with \(s \neq s'\) was varied between 0 and 2. In all these simulation cases, the diagonalization of the hardening matrix \(r=0\) method was used. Additionally, the predictions of the standard EPSC are also presented for the purpose of comparison. The dislocation-based hardening law parameters were slightly adjusted for each simulation case. The parameters are given in Table 3. The backstress parameters were kept the same, as presented in Table 1b. Figure 9 compares the experimental and simulated ratio of the true stress in tensile direction for the three studied directions to the true stress in tension along the RD sample at a true strain of 0.18. It can be seen
Fig. 9. True stress at a true strain of 0.18 predicted in tension along the three directions as indicated on the x-axis normalized by the tensile true stress in RD. The corresponding experimental results are presented to facilitate the comparison.

Table 3. Constitutive parameters for the evolution of slip resistance for \{111\}(\overline{1}0) slip mode in AA6022-T4.

<table>
<thead>
<tr>
<th>$L^{ss}$</th>
<th>$L^{ss'}$</th>
<th>$g^{ss}$</th>
<th>$g^{ss'}$</th>
<th>$\tau_0$ [MPa]</th>
<th>$k_1 [m^{-1}]$</th>
<th>$g$</th>
<th>$D$ [MPa]</th>
<th>$q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 0 1 0 60</td>
<td>3.0 x 10^8</td>
<td>0.1176</td>
<td>100</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 0.5 1 0 60</td>
<td>1.6 x 10^8</td>
<td>0.0866</td>
<td>100</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 1 1 0 58</td>
<td>1.3 x 10^8</td>
<td>0.0706</td>
<td>100</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 2 1 0 56</td>
<td>1.1 x 10^8</td>
<td>0.0523</td>
<td>100</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

that the flow stress ratio for 45° and TD is decreasing with the latent hardening coefficients. Anisotropy in flaw stress follows the experimental trend ($\sigma_{RD} > \sigma_{45} > \sigma_{TD}$) better when the latent hardening coefficient is $\geq 1$. In addition, Fig. 9 shows the effect of diagonalization of hardening matrix on anisotropy. The effect can be appreciated by focusing on the predictions from the standard EPSC and the predictions from the diagonalization of the hardening matrix for constants $L^{ss'} = 0.99$ and $L^{ss} = 1$. The comparison reveals that even with similar latent hardening, the diagonalization of
hardening matrix produces the desired trend in the flow stress anisotropy. Evidently, the experimental values adopted from [13] further improve the predictions.

4.3 Improved predictions using the interaction matrix, $g^{ss'}$

The predictions presented thus far considered $g^{ss'}$ as diagonal matrix populated with the values of unity on the diagonal. The rate of dislocation generation per slip system is dependent on dislocation density in itself and other slip systems in a complex manner [122]. In the dislocation evolution law, the interdependence between slip systems in terms of generation of dislocations can be implemented by increasing the off-diagonal terms in $g^{ss'}$. The $g^{ss'}$ controls the dislocation evolution rate in the same way the $L^{ss'}$ controls the slip resistance. The hardening rate of a slip system, defined with entries of hardening matrix in appendix A, is proportional to dislocation evolution rate. Therefore, the rate of hardening of all slip systems due to shearing on an active slip system is controlled in part by $g^{ss'}$ interaction matrix. The strength interaction matrix, $L^{ss'}$, remained the same, i.e. the self-hardening and the coplanar interactions are unity while all the remaining terms are 1.4. The effect of increasing off-diagonal terms in matrix $g^{ss'}$ on anisotropy in flow stress is shown in Fig. 10a. The predictions improve with increasing the magnitude of the $g^{ss'}$ off-diagonal entries but then saturate. No appreciable improvements are obtained after a value of 1 for the off-diagonal entries. The empirical backstress law is still used with the parameters given in Table 1b. As always, the hardening law parameters were adjusted to obtain the best fit to the measured data and are given in Table 4. The fits to true stress-true strain curves and the predictions of r-ratio are given in Figs. 10b and c, respectively. Evidently, the model
successfully captures the evolution of anisotropy. We regard the predicted trends as good. We note that introducing the off-diagonal terms in the matrix $g^{ss'}$ within the standard EPSC can have some positive effect on the flow stress anisotropy, while the $r$-ratio predictions become worse.

![Diagram](image)

**Fig 10.** (a) True stress at a true strain of 0.18 predicted in tension along the three directions as indicated on the x-axis normalized by the tensile true stress in RD. The corresponding experimental results are presented to facilitate the comparison. (a) Simulated compared with the measured true stress-true strain curves and (b) simulated compared with the measured $r$-ratio for AA6022-T4.
Table 4. Constitutive parameters for the evolution of slip resistance for \{111\}(1\overline{1}0) slip mode in AA6022-T4. The (Kocks and Brown, 1966) refers to setting self and coplanar interactions between slip systems to 1.0, while all other interactions are defined to be 1.4.

<table>
<thead>
<tr>
<th>$L^{ss}$</th>
<th>$L^{ss'}$</th>
<th>$g^{ss}$</th>
<th>$g^{ss'}$</th>
<th>$\tau_0$ [MPa]</th>
<th>$k_1$ $[m^{-1}]$</th>
<th>$g$</th>
<th>$D$ [MPa]</th>
<th>$q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>56</td>
<td>$1.3 \times 10^8$</td>
<td>0.0618</td>
<td>100</td>
<td>8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>56</td>
<td>$0.65 \times 10^8$</td>
<td>0.0294</td>
<td>100</td>
<td>8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(Kocks and Brown, 1966)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>56</td>
<td>$0.5 \times 10^8$</td>
<td>0.022</td>
<td>100</td>
<td>8</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

In summary, the simulation results reveal that the strength interaction matrix, $L^{ss'}$, and the interaction matrix defining the rate of dislocation generation, $g^{ss'}$, for the given crystallographic texture and its evolution have a significant effect on the observed anisotropy in stress-strain response of AA6022-T4.

4.4 Large strain cyclic plasticity predictions for AA6022-T4

Finally, the predictive characteristics of the model are evaluated on the large strain cyclic data for the material. The presented dislocation density-based hardening along with the empirical backstress model with the parameters given in Tables 4 and 1b has been utilized in the EPSC model with the diagonalization of the hardening matrix procedure for these calculations. The reversibility parameter was set to $p = 0.2$ (Eqs. 21-23). Figure 11 shows the predictions. It can be seen that the model using the single set of parameters is capable of predicting the non-linear unloading, the BE, and the hardening rates upon loading in the reverse direction of the material with reasonable accuracy. Therefore, the EPSC integrating the diagonalization of the hardening matrix is still able to produce similar predictions of the cyclic response to the standard EPSC [123].
Fig 11. Comparison of measured (solid lines) and predicted (dashed lines) large strain cyclic tension-compression response along RD. The predictions are based on the new EPSC model with diagonalization of hardening matrix.

5. Conclusions

This paper extends a recently developed dislocation-based hardening law within the EPSC homogenization [53, 54] to incorporate the latent hardening effects for the prediction of plastic anisotropy of polycrystalline metals. The new implementation overcomes an issue in the self-consistent formulation with latent hardening arising when experimentally measured latent hardening constants are used. The main issue is identified to be the loss of ellipticity of macroscopic tangent modulus caused by the loss of ellipticity of single crystal tangent modulus. The new method takes the advantage of a new solution procedure for single crystal stress increment relying on the singular value decomposition and a penalty method to solve for shear increments and a set of active slip systems, respectively. The method, termed the diagonalization of hardening matrix, is compared with the regularized Schmid law method, which does not have the issue with the loss of ellipticity. The comparison shows that the new implementation is closer
in terms of stress-strain predictions to the original EPSC formulation than the regularized Schmid law, leading to more accurate predictions. Moreover, the new method is much more computationally efficient.

Effect of latent hardening on plastic anisotropy in the mechanical response of AA6022-T4 is studied using the developed crystallographic modeling framework. The proposed method for overcoming the loss of ellipticity, which facilitates the use of the experimentally determined latent hardening coefficients for aluminum reported in [13], predicts the correct anisotropy in the stress-strain response of the studied material. Thus, the latent hardening, along with crystallographic texture evolution, are found to control plastic anisotropy in AA6022-T4. Moreover, the model improves the predictions of r-ratio evolution with plastic strain. Finally, the proposed model is able to predict the large strain cyclic plasticity behavior of the material.

Acknowledgments

This work is based upon projects supported by the US National Science Foundation under grants CMMI-1301081 and CMMI-1650641.

Appendix A

Entries of the hardening matrix are partial derivatives of slip resistance given with relation (17) with respect to shear strain on slip systems:

\[ h_{ss'} = \frac{\partial \tau_c}{\partial \gamma_{ss'}} = \frac{\partial \tau_0}{\partial \gamma_{ss'}} + \frac{\partial \tau_{\text{forest}}}{\partial \gamma_{ss'}} + \frac{\partial \tau_{\text{debris}}}{\partial \gamma_{ss'}}. \] (A1)
The index $s'$ goes over all active slip systems. Since the initial slip resistance, $\tau_0^\alpha$, is a constant its derivative vanish, while derivatives of the forest and debris contributions to slip resistance are:

$$\frac{\partial \tau_{\text{forest}}^s}{\partial \gamma^{s'}} = \frac{\partial \tau_{\text{forest}}^s}{\partial \rho_{\text{tot}}^{s'}} \frac{1}{2 \sum_{s'} L_{ss'} \rho_{\text{tot}}^{s'}} \left( \frac{\partial \rho_{\text{for}}^{s'}}{\partial \gamma^{s'}} + \frac{\partial \rho_{\text{rev}}^{s'}}{\partial \gamma^{s'}} + \frac{\partial \rho_{\text{rev}}^{-}}{\partial \gamma^{s'}} \right), \quad (A2)$$

$$\frac{\partial \tau_{\text{debris}}^s}{\partial \gamma^{s'}} = \frac{\partial \tau_{\text{debris}}^s}{\partial \rho_{\text{deb}}^{s'}} = -k_{\text{deb}}^\alpha b^\alpha \left( \log \left( b^\alpha \sqrt{\rho_{\text{deb}}} \right) + 1 \right) \frac{1}{2 \sqrt{\rho_{\text{deb}}}} \frac{\partial \rho_{\text{deb}}^{s'}}{\partial \gamma^{s'}}. \quad (A3)$$

The derivatives of forward, reversible, and debris dislocation densities with respect to shear strain are provided with Eqs. (21a-23b, 26) respectively.

Similarly, entries of the backstress matrix are partial derivatives of backstress given with relation (27) with respect to shear strain on slip systems:

$$h_{bs}^{ss'} = \frac{\partial \tau_{bs}^s}{\partial \gamma^{s'}} = \begin{cases} \frac{\partial \tau_{bs,sys}^s}{\partial \gamma^{s'}} & \text{if } s = s' \\ 2 m^s \cdot m^{s'} \frac{\partial \tau_{bs,sys}^*}{\partial \gamma^{s'}} & \text{if } s \neq s' \end{cases} \quad (A4)$$

where $s'$ goes over set of active slip systems. Using the relation (28) the derivative

$$\frac{\partial \tau_{bs,sys}^{s'}}{\partial \gamma^{s'}}$$

is:

$$\frac{\partial \tau_{bs,sys}^{s'}}{\partial \gamma^{s'}} = \begin{cases} \frac{\partial \tau_{bs,sys}^{s'}}{\partial \gamma^{s'}} & \text{if } \tau_{bs,sys}^{s'} > 0 \\ 0 & \text{if } \tau_{bs,sys}^{s'} > 0 \end{cases} \quad (A5)$$

Next we define the derivative of slip system backstress sources, $\frac{\partial \tau_{bs,sys}^{s'}}{\partial \gamma^{s'}}$. In the case of shearing in $s^*$ direction, $d\gamma^{s^*} > 0$, with $\tau_{bs}^{s^*} \geq 0$:  

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\[ \frac{\partial \tau_{bs,sys}^{s+}}{\partial y^s} = \tau_{bs}^{sat} \nu \exp(-\nu \gamma^s), \quad (A6) \]

\[ \frac{\partial \tau_{bs,sys}^{s-}}{\partial y^s} = -A \frac{\partial \tau_{bs,sys}^{s+}}{\partial y^s}. \quad (A7) \]

The derivative of slip system backstress source in case of shearing in \( s^+ \) direction, \( d\gamma^s > 0 \), with \( \tau_{bs,sys}^{s+} < 0 \) is:

\[ \frac{\partial \tau_{bs,sys}^{s+}}{\partial y^s} = \frac{(A+1) \tau_{bs}^{sat}}{\gamma_b} \exp \left( -\frac{\gamma^s}{\gamma_b} \right), \quad (A8) \]

\[ \frac{\partial \tau_{bs,sys}^{s-}}{\partial y^s} = A \frac{\partial \tau_{bs,sys}^{s+}}{\partial y^s}. \quad (A9) \]

**Appendix B**

The purpose of integration algorithm is to find an increment in plastic multiplier, \( \Delta \lambda \), for a given increment in a crystal strain, \( \Delta \varepsilon^c \). In the semi-implicit integration procedure [116] the normal to yield surface is evaluated at the beginning of the time increment by calculating:

\[ \hat{n}_t = \frac{1}{\sum_s \left( \frac{\sigma_t \cdot m_t^s}{\tau_{c,t}^{s+} + \tau_{bs,t}^{s+}} \right)^{2N-1}} \sum_s \left( \frac{\sigma_t \cdot m_t^s}{\tau_{c,t}^{s+} + \tau_{bs,t}^{s+}} \right)^{2N-1} \frac{1}{\tau_{c,t}^{s+} + \tau_{bs,t}^{s+}} m_t^s. \quad (B1) \]

All variables having subscript \( t \) are written at instant \( t \) and are known. Therefore, in Eq. (B1), all variables on the right hand side are known, and \( \hat{n}_t \) can simply be calculated. The yield function is written at the end of the time increment:

\[ f_{t+\Delta t} = \left( \sum_s \left( \frac{\sigma_{t+\Delta t} \cdot m_t^s}{\tau_{c,t+\Delta t}^{s+} + \tau_{bs,t+\Delta t}^{s+}} \right)^{2N} \right)^{\frac{1}{2N}} - 1 = 0, \quad (B2) \]
with:

\[ \sigma_{t+\Delta t}^c = \sigma_t^c + \Delta \sigma^c = \sigma_t^c + C^c(\Delta \varepsilon^c - \Delta \lambda \hat{n}) \],

\[ \tau_{c,t+\Delta t}^s = \tau_{c,t}^s + \sum_{s'} h_{t}^{ss'} \Delta \gamma^{s'} = \tau_{c,t}^s + \Delta \lambda \sum_{s'} h_{t}^{ss'} \hat{n}_{t}^{s'}, \] (B3)

\[ \tau_{b,s,t+\Delta t}^s = \tau_{b,s,t}^s + \sum_{s'} h_{bs,t}^{ss'} \Delta \gamma^{s'} = \tau_{b,s,t}^s + \Delta \lambda \sum_{s'} h_{bs,t}^{ss'} \hat{n}_{t}^{s'}, \] (B4)

where \( \Delta \lambda \) is the increment in plastic multiplier. (B2) is a non-linear equation with \( \Delta \lambda \) as unknown. Newton method is used to solve for \( \Delta \lambda \). Next, increments in shear strain on slip systems, slip resistance, plastic strain, and stress can be calculated and total variables updated.

The consistent tangent operator is:

\[ \frac{\partial \Delta \sigma^c}{\partial \Delta \varepsilon^c} = \frac{\partial}{\partial \Delta \varepsilon^c} [C^c(\Delta \varepsilon^c - \Delta \lambda \hat{n})] = C^c - C^c \hat{n} \otimes \frac{\partial \Delta \lambda}{\partial \Delta \varepsilon^c}, \] (B6)

\[ \frac{\partial \Delta \lambda}{\partial \Delta \varepsilon^c} \]

can be calculated by taking the derivative of relation (B2):

\[ \frac{1}{2N} \left( \sum_s \left( \frac{\sigma_{t+\Delta t}^c m_t^s}{(\tau_{c,t+\Delta t}^s + \tau_{bs,t+\Delta t}^s)^2} \right) \right)^{1-2N} \left( \sum_s \left( \frac{\sigma_{t+\Delta t}^c m_t^s}{(\tau_{c,t+\Delta t}^s + \tau_{bs,t+\Delta t}^s)^2} \right) \right)^{2N-1} \frac{1}{(\tau_{c,t+\Delta t}^s + \tau_{bs,t+\Delta t}^s)^2} \frac{\partial (\sigma_{t+\Delta t}^c m_t^s)}{\partial \Delta \varepsilon^c} = 0, \] (B7)

where:

\[ \frac{\partial (\sigma_{t+\Delta t}^c m_t^s)}{\partial \Delta \varepsilon^c} = m_t^s C^c - m_t^s C^c \hat{n}_{t} \otimes \frac{\partial \Delta \lambda}{\partial \Delta \varepsilon^c}, \] (B8)

\[ \frac{\partial (\tau_{c,t+\Delta t}^s + \tau_{bs,t+\Delta t}^s)}{\partial \Delta \varepsilon^c} = \frac{\partial \Delta \lambda}{\partial \Delta \varepsilon^c} \sum_{s'} (h_{t}^{ss'} + h_{bs,t}^{ss'} \hat{n}_{t}^{s'}). \] (B9)
From (B7), $\frac{\partial \Delta \Lambda}{\partial \Delta \varepsilon^c}$ can be expressed as:

$$
\frac{\partial \Delta \Lambda}{\partial \Delta \varepsilon^c} = 
\left( \sum_s \left( \frac{\sigma_{i+\Delta t}^c m_i^s}{r_{i+\Delta t}^s + r_{bs,t+\Delta t}^s} \right) \right) \frac{2^{N-1}}{1} \left( \sum_s \left( \frac{\sigma_{i+\Delta t}^c m_i^s}{r_{i+\Delta t}^s + r_{bs,t+\Delta t}^s} \right) \right) \frac{1}{1}
\left( m_i^s \hat{c} \frac{\partial \Delta \Lambda}{\partial \Delta \varepsilon^c} \right) \left( m_i^s \hat{c} + \text{const.} \right)
\left( \sum_s \left( h_{t+\Delta t}^{ss} + h_{bs,t}^{ss} \right) \right) \left( \sum_s \left( h_{t+\Delta t}^{ss} + h_{bs,t}^{ss} \right) \right) 
$$

(B10)

**Appendix C**

Constitutive relations in presence of eigenstrain for single crystal and polycrystal, respectively, are:

$$
\Delta \sigma^c = L^c (\Delta \varepsilon^c - \Delta \varepsilon^{*c}), \quad (C1)
$$

$$
\Delta \sigma = L (\Delta \varepsilon - \Delta \varepsilon^*), \quad (C2)
$$

where $L^c = \frac{\partial \Delta \sigma^c}{\partial \Delta \varepsilon^c}$ is consistent tangent operator. Interaction equation for inhomogeneity inside the matrix is:

$$
\Delta \sigma^c - \Delta \sigma = -L^* (\Delta \varepsilon^c - \Delta \varepsilon), \quad (C3)
$$

with $L^* = L (S^{c-1} - 1)$. Replacing constitutive relation inside the interaction equation gives:

$$
L^c (\Delta \varepsilon^c - \Delta \varepsilon^{*c}) - L (\Delta \varepsilon - \Delta \varepsilon^*) = -L^* (\Delta \varepsilon^c - \Delta \varepsilon). \quad (C4)
$$

From relation (C4) increment in strain can be expressed as:

$$
\Delta \varepsilon^c = A^c \Delta \varepsilon^{ref} + a^c, \quad (C5)
$$
with

\[
A^c = (L^c + L^*)^{-1}(L + L^*),
\]

\[
a^c = (L^c + L^*)^{-1}(L^c \Delta \varepsilon^c - L \Delta \varepsilon^*),
\]

where \(\Delta \varepsilon^{ref}\) is the unknown reference increment in strain [124]. Using the condition that the volume average of single crystal increments in strain is equal to the macroscopic increment in strain gives the expression for reference strain increment:

\[
\Delta \varepsilon = \langle \Delta \varepsilon^c \rangle = (A^c)\Delta \varepsilon^{ref} + \langle a^c \rangle \to \Delta \varepsilon^{ref} = (A^c)^{-1}\Delta \varepsilon - \langle A^c \rangle^{-1}\langle a^c \rangle.
\]

(C8)

In a similar manner, the volume average of single crystal increments in stress is equal to the macroscopic increment in stress:

\[
\Delta \sigma = \langle \Delta \sigma^c \rangle = (L^c A^c)\langle A^c \rangle^{-1}\Delta \varepsilon - \langle L^c A^c \rangle\langle A^c \rangle^{-1}\langle a^c \rangle + \langle L^c(a^c - \Delta \varepsilon^c) \rangle.
\]

(C9)

By comparing relation (C9) with (C2) we can identify macroscopic tangent stiffness and eigenstrain:

\[
L = (L^c A^c)\langle A^c \rangle^{-1},
\]

(C10)

\[
\Delta \varepsilon^* = \langle a^c \rangle - L^{-1}(L^c(a^c - \Delta \varepsilon^c)).
\]

(C11)

References


CHAPTER 6:

Polycrystal plasticity modeling of mechanical fields and microstructure evolution during simple tension and CBT of AA6022-T4

1. Introduction

Sufficient formability, described with the forming limit curve (FLC), is required from materials used in sheet metal forming processes. Advanced alloys, such as aluminum alloy AA6022-T4 and dual phase steel DP780, poses limited formability. During forming of materials with limited formability a plastic instability, i.e. necking, may occur, leading to excessive plastic deformation in small regions of the part and, in turn, fracture. Changing the deformation history to reach the final part shape by altering the forming process, can postpone the deformation localization and fracture. For instance, introduction of drawbeads to sheet metal forming is known to increase strain to failure [1]. During drawing through drawbeads, the sheet experiences simultaneous bending and tension. Such mechanism is referred to as bending under tension (BUT). A class of forming processes, termed incremental sheet forming (ISF) processes, allows forming beyond FLC [2]. In the ISF a small volume of a part at a given time instant undergoes plastic deformation. One of the possible stabilizing mechanisms acting during ISF is BUT [2]. The BUT mechanism can be isolated and studied by performing the continues bending under tension (CBT) test, first proposed in [3]. Superimposing bending, introduced by three rollers positioned as shown in Fig 1, to the simple tension (ST) produces the CBT test configuration. During the CBT test, constant velocity is applied at
right end of the specimen, referred to as the crosshead velocity, while the left end is clamped, see Fig 1. During CBT cycles rollers travel from one end of the gauge section to the other. The described CBT test set up allows specimens to experience larger elongation to fracture than during the ST [3-6]. Besides studying the CBT test for purpose of improving the sheet metal forming processes, the CBT test can provide insight into material behavior at large strains [3].

Understanding the mechanics of the CBT test and the material behavior at large strains requires experimental investigation and modeling. There have been several experimental studies of the mechanical response of different materials during the CBT test [4-6]. The effect of the CBT processing on the material stress-strain response, texture evolution and damage evolution was experimentally characterized in [7]. Mechanics of the CBT process was analyzed in [8]. Furthermore, several numerical models of the CBT process have been presented in literature [5, 9, 10]. Numerical models with yield surface based constitutive laws have been able to predict the mechanical response during the CBT test, but are unable to give insight into the microstructure evolution. Furthermore, the material model needs to be calibrated with the cyclic mechanical response, resembling strain paths experienced by material points during the CBT process, in order to get accurate predictions [9]. The experimental data for such strain paths is not readily available in literature. Therefore, material models with advanced predictive capabilities, such as crystal plasticity micromechanical models, should be favored when modelling the CBT processes.

The objectives of this chapter are to: (1) calibrate the elasto-plastic self-consistent (EPSC) material model for aluminum alloy AA6022-T4, developed in
preceding chapters, with the cyclic experimental data relevant for the CBT process, (2) perform a finite element (FE) simulation of the CBT test with the EPSC material model, (3) compare the model output with experimental measurements and provide some insight into the CBT process and material behavior.

![Schematic of the continuous bending under tension (CBT) loading](image)

**Fig. 1.** Schematic of the continuous bending under tension (CBT) loading [7].

**2. Material characterization, mechanical testing and model calibration**

The material used in this study is a solid solution strengthened aluminum alloy, labeled AA6022-T4, with Si (wt. % 1.21) and Mg (wt. % 1.21) as primary alloying elements and small content of precipitates. The initial crystallographic texture of the as received material is shown in Fig. 2. The texture was reconstructed from a large EBSD scan. AA6022-T4 was extensively studied in previous studies [11, 12], and more information about the material and its mechanical behavior is available there. Samples of the received material in form of a sheet of 1 mm thickness were subjected to CBT, tensile and cyclic tests.
The experimental setup for CBT, shown in Fig 3, has been developed and presented in [5, 6] and reader is referred to these references for details on the CBT machine design. On contrary to previous designs of the CBT test, where the carriage with a set of rollers traverses along the specimen being pulled by a universal testing machine [3, 4], in current study rollers are stationary, while the specimen with tensile loading apparatus is placed on the traversing carriage. The pulling force to achieve a constant pulling velocity applied to one end of the specimen is recorded with load cells. The stationary rollers setup allows testing of sheets and use of the Digital Image Correlation (DIC) technique for measuring strain fields on the specimen. These additional features will be explored in future work. The results in this study are reported for a specimen in form of a strip.

Fig 2. Pole figures showing measured texture of as received AA6022-T4.

The material mechanical response was further characterized with standard tensile tests, shown in Fig 4a with full lines. Tension tests were performed in rolling direction (RD), transverse direction (TD) and 45 degree to RD direction, showing the in-plane anisotropy [13]. A stress-strain curve to large strain is shown in Fig 4b. The curve was presented in [14] and is evaluated by the bulge test. Since the CBT test suppresses
necking, the strain in tension direction in some regions of the CBT specimen exceeds the maximum strain recorded during regular tension test. The behavior of the material at such large strains needs to be accurately simulated for modeling of the CBT test and the curve shown in Fig 4b will be used to verify that the model extrapolated curve to large strain is reasonable. The stress level of the experimental curve from the bulge test is somewhat different both in hardening rate and yield stress than the rest of the data. The deviation is attributed to the simplifications in evaluation of the stress-strain curve from the actual measurements from the bulge test and any possible differences in composition and thermo-mechanical processing history of tested material in [14] compared to the material from [13].

![Experimental setup for CBT test.](image)

**Fig. 3.** Experimental set up for CBT test.

Next, cyclic experiments were performed, designed to provide insight into the mechanical behavior of the material during strain paths characteristic of the CBT test [9,
The cyclic plasticity experiments were performed at Tokyo University of Agriculture & Technology [16]. The testing setup ensures lateral support of the specimen with constant pressure to avoid buckling during compressive region of cyclic loading [16]. Appropriate lubrication is applied to specimen to reduce the effect of friction between the specimen and lateral supports. The measured cyclic response of AA6022-T4 is shown in Figure 5 with full lines.

![Comparison of measured (solid lines) and simulated (dashed lines): (a) true stress-true strain curves for simple tension in RD, TD and 45 directions and (b) true stress-true strain curves for simple tension to large strain, where experimental data was taken from [14].](image)

**Fig. 4.** Comparison of measured (solid lines) and simulated (dashed lines): (a) true stress-true strain curves for simple tension in RD, TD and 45 directions and (b) true stress-true strain curves for simple tension to large strain, where experimental data was taken from [14].

The model used in this study is elasto-plastic self-consistent model coupled with finite elements (FE-EPSC) presented in [17]. The EPSC model input consists of: crystal orientations of the representative volume element (RVE), single crystal elastic constants, slip system geometry and hardening law parameters. The crystal orientations in the RVE were generated from measured texture shown in Fig 2. The measured texture was reduced to a sufficiently small number of orientations, while preserving the important features governing the mechanical response, using an algorithm developed in
Fig. 5. Measured (full lines) and simulated (dashed lines) cyclic response of AA6022-T4.

Table 1. Constitutive parameters for the evolution of slip resistance for \{111\}(1\bar{1}0) slip mode in AA6022-T4.

<table>
<thead>
<tr>
<th>( l_{\text{coplanar}} )</th>
<th>( l_{\text{non-coplanar}} )</th>
<th>( g^{ss} )</th>
<th>( g^{ss'} )</th>
<th>( \tau_0 ) [MPa]</th>
<th>( k_1 ) [m(^{-1})]</th>
<th>( g )</th>
<th>( D ) [MPa]</th>
<th>( q )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>1.4</td>
<td>1</td>
<td>0</td>
<td>57</td>
<td>1.7 \times 10^8</td>
<td>0.055</td>
<td>100</td>
<td>4</td>
</tr>
</tbody>
</table>

Table 2. Parameters for the evolution of slip system kinematic backstress in AA6022-T4.

<table>
<thead>
<tr>
<th>( \tau_{bs}^{sat} ) [MPa]</th>
<th>( v )</th>
<th>( \gamma_b )</th>
<th>( A )</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>560</td>
<td>0.001</td>
<td>1</td>
</tr>
</tbody>
</table>
The representation of measured texture with minimum number of orientations significantly reduces the computational time, since the EPSC computational time is proportional to the number of crystals used as input. The single crystal elastic constants of Al are: $C_{11} = 108.2 \, MPa$, $C_{44} = 28.5 \, MPa$ and $C_{12} = 61.3 \, MPa$ [19]. The slip systems belonging to $\langle 110 \rangle \{ 111 \}$ slip family, active in face centered cubic (fcc) materials, are allowed to activate and accumulate shear strain in the EPSC model. The hardening law parameters were calibrated by comparing the simulated and measured stress-strain curves for both monotonic tension tests and cyclic tests. The best fits to experimental stress-strain curves are shown with dashed lines in Figs 4 and 5, while the fitting parameters of the model are reported in Tables 1 and 2. The reported parameters are somewhat different from the ones calibrated in [12, 17] due to reduced texture and consideration of additional cyclic and monotonic stress-strain curves in fitting procedure. In addition, a simplified backstress evolution law, described in appendix A, is utilized.

3. The CBT simulation with FE-EPSC

The FE model of the CBT test in Abaqus is shown in Fig 6a. The specimen gauge thickness and width are 1 mm and 11.75 mm, respectively, while the starting gauge length disturbed by rollers is close to 190 mm. One half of the specimen is modeled due to the symmetry of applied loads and specimen geometry. The model consists of 2712 continuum shell elements (SC8R in Abaqus notation [20]). The section behavior of the shell element is calculated by integrating in the shell thickness direction. The numerical integration is performed using 5 integration points through thickness. The top and the bottom surface and section integration points are identified in Fig 6b. The
rollers were modeled as analytical rigid surfaces. The friction coefficient between rollers and the specimen was set to 0.17.

The specimen was clamped at the left end, referring to Fig 6a, while constant velocity is applied to the right end of the specimen. First, the top roller is lowered to achieve the desired bending depth of 2.5 mm, see Fig 6c. The radius of rollers is 12.7 mm. One CBT cycle includes motion of rollers, with velocity of 66 mm/s, from left end of the gauge section to the right end, and then back to their starting position at the left end of the gauge section. The first CBT cycle is run with 0 crosshead velocity, while subsequent 7.5 cycles are run with constant crosshead velocity of 1.182 mm/s.

![Diagram](image)

**Fig. 6.** (a) FE mesh and model set up, (b) identification of through thickness points and (c) definition of bending depth.
The simulation was performed with user defined material behavior, implemented through UMAT subroutine [17]. The predicted and measured forces applied to the right end of the specimen to maintain the constant crosshead velocity are plotted against the crosshead displacement in Fig 7a. The agreement between the experiment and the simulation is very good up to displacement of around 30 mm, after which the simulated response starts to deviate more from the experiment. The force displacement profile is correlated with roller velocity [5]. Peaks in force correspond to the end of acceleration period of rollers. The decrease of the force after peak value occurs during motion of rollers with constant velocity from one end of the gauge section to the other. The minimum in force corresponds to the end of constant velocity period of rollers and the start of roller deceleration, close to the end of the gauge section.

The texture after total of 12 CBT cycles in RD was measured in [7]. The bending depth, crosshead velocity and roller velocity were 1.75, 0.86 mm/s and 66 mm/s, respectively. The measured texture after 12 CBT cycles, corresponding to crosshead displacement of 54.92 mm, is compared with the predicted texture by the model after total of 8.5 CBT cycles, corresponding to crosshead displacement of 52.45 mm, in Fig 7b. The simulated texture is plotted for all through thickness points of an element in the middle of the specimen in width and axial directions. The comparison of the starting texture with the texture after 12 CBT cycles shows formation of 〈111〉 fiber and strengthening of 〈001〉 fiber in the texture after 12 CBT cycles. Similar trends are observed in predicted texture after 8.5 CBT cycles, but with slightly lower intensity. The comparison between the measured and the predicted texture is semi-quantitative, since
they have been recorded after different number of CBT cycles performed with different parameters, but at similar displacements.

![Graph and images](image)

**Fig. 7.** (a) The measured and simulated force displacement profile during the CBT test. (b) The measured texture after 12 CBT cycles and the simulated texture after 8.5 CBT cycles.
From the comparison between the simulation and the experiment, we conclude that the model is capable of capturing the experimentally observed trends in the mechanical response and the texture evolution during the CBT process.

4. **CBT vs simple tension (ST)**

Accurate predictions of the mechanical response and the texture evolution give some confidence in accuracy of model predictions of other quantities, not easily accessible to experimental measurement. In this section, we analyze the mechanisms of plastic deformation during the CBT process, in comparison with the simple tension (ST). In addition, we compare model predictions of material state variables between the CBT and the ST at corresponding levels of plastic strain.

The stress state in the gauge section of the specimen during the ST is uniform. On the other hand, in the CBT gauge section, the stress state is non-uniform. Three external loads are acting on the CBT specimen: (1) the force applied at the end of the specimen to achieve constant crosshead velocity causing the tensile stress, (2) traction on the surface of the specimen in contact with rollers, introducing bending stresses in the proximity of rollers and (3) reaction moments originating from the constraint of the grips, preventing the bending of the specimen due to the through thickness gradient in axial plastic strain. Internal stress field originating from inhomogeneous plastic deformation at both macroscopic and microscopic scale interacts with external loads, causing plastic deformation in region around rollers, while the rest of the specimen is elastic. It is the division of the specimen volume into small plastic region and remaining elastic region, by presence of rollers, that suppresses the strain localization in the CBT. Motion of rollers “moves” the plastic region across the specimen causing sequential
plastic deformation of the specimen gauge section, as opposed to the ST where the plastic deformation occurs in parallel in all regions of the gauge section. The plastic deformation occurs in parallel only in regions in proximity of the rollers during the CBT. The sequential plastic deformation of the gauge section breaks the interaction between plastically deforming regions. The presence of a weaker region, therefore, does not affect other regions and their plastic deformation in the CBT. On contrary, presence of a weaker region in the ST causes all other regions to unload at the moment neck forms in the weaker region.

![Diagram of finite element 1287](image)

**Fig. 8.** Identification of finite element 1287, used to analyze the CBT deformation process

The specimen gauge section can be divided into three regions, labeled: 1x, 2x and 3x. The basis for 1x, 2x and 3x division is the number of rollers that visit the region during the course of the CBT test. 1x region of the gauge section is located at ends of the gauge section and comes into contact with only one roller during the CBT test. 3x region comes into contact with all three rollers and is located in the central region of the gauge section, while 2x region comes into contact with two rollers and is located...
between 1x and 3x region. A material point in 3x region of the CBT specimen experiences a complex stress/strain history, unlike the points in the ST. Furthermore, there is a stress/strain gradient in thickness and width direction in the 3x region of the CBT specimen. An arbitrary element with number 1287, located in the 3x region in the middle of the specimen with respect to width direction, is identified in Fig 8. Fig 9a shows the true axial strain, $\varepsilon_{11}$, the true axial plastic strain, $\varepsilon_{11}^{pl}$ and the true axial stress, $\sigma_{11}$, as rollers move over element 1287 during the 1st half of the 3rd CBT cycle. The labeling of section points of the element 1287 is consistent with Fig 6b. Before rollers visit the region of interest, the bottom point (SP5) has tensile axial stress, while all other points (SP1-SP4) have compressive axial stress. The axial strain is roughly the same for all points. Since the specimen is elastic outside of the region engaged by rollers, we can say that the observed stress distribution is a superposition of the tensile stress from the pulling force, the stress from the bending moment induced by grips and internal stress field from inhomogeneous plastic deformation. The bending moment is responsible for the characteristic shape of unloaded specimens observed in [5]. The true strain and stress in direction 22 are shown in Fig 9b. Once the first roller moves over the element 1287 it introduces additional bending compressive axial strain to the bottom point (SP5) and the tensile strain to the top point (SP1). The 2nd roller has opposite effect and puts the top point into compression and the bottom point in tension. Passage of the third roller has similar effect as the passage of the first roller. Examination of the plastic strain in axial direction, plotted in Fig 9a, shows the plastic deformation in section points occurs during the passage of the 2nd and the 3rd roller. The top and the bottom points experience both compressive and tensile plastic deformation.
Fig. 9. (a) True strain, true plastic strain and true stress in direction 11 and (b) true strain and true stress in direction 22, for all section points within element 1287, during passage of all three rollers.
in axial direction, i.e. strain path reversals, during the passage of the 2nd and the 3rd roller. Accumulation of tensile strain in the axial direction is accompanied by tensile stresses in axial (stress component 11) and width (stress component 22) direction. On the other hand, three section points, between the top and the bottom point, experience only tensile plastic deformation in axial direction. The normal stress in the width direction is positive during the plastic deformation of section points SP3 and SP4, while the SP2 undergoes both tensile and compressive stresses in the width direction during the plastic deformation, see Fig 9.

The spatial distribution of the true axial strain along the symmetry line, indicated in Fig 8, is shown in Fig 10. The strain in the region disturbed by all three rollers is shown as the 3x region, while the regions visited by two and three rollers are labeled as 2x and 1x regions in Fig 10, respectively. The strain distribution in 3x region is close to uniform for first 5 CBT cycles, after which strain starts to localize close to the transition between 3x and 2x region. The predicted strain localization position matches with experimental measurements of axial strain profile along the length of the specimen shown in [6] and numerical predictions from [5]. Furthermore, the CBT specimens fracture at these strain localizations [5].

The difference in the stress/strain history between the CBT and the ST governs the difference in microstructure evolution. Comparison between the CBT and the ST is performed at the same level of axial plastic strain in terms of relevant macroscopic and microstructural variables. An arbitrary element in 3x region with number 1503, located in the middle of the specimen with respect to axial and width direction, is used for the
Fig. 10. True axial strain at nodes positioned along the center of the specimen i.e. along the symmetry line, plotted against the normalized x coordinate of nodes defining relative position of a node within the region disturbed by rollers. The axial strain profiles are plotted after every CBT cycle, excluding the first one. Regions visited by one roller (1x), two rollers (2x) and three rollers (3x) are indicated.

Comparison of the CBT deformation process with the ST. All 5 through thickness points are compared with the ST. The comparison is performed after 5.5 CBT cycles. The average axial plastic strain over all section points through thickness is 0.172 after 5.5 CBT cycles. The ST was as well simulated to the axial plastic strain of 0.172. Fig 11 compares the state for the CBT after 5.5 cycles with the ST state at 0.172 plastic strain. The compared quantities in Fig 11 are:

1. the equivalent plastic strain, $\varepsilon^{pl,eq}$.

2. the volume average true plastic strain over grains i.e. macroscopic plastic strain, $\varepsilon_{ij}^{pl}$. 
3. the deviation of grain plastic strain components, $\varepsilon_{ij}^{pl,c}$, from the macroscopic plastic strain, $\varepsilon_{ij}^{pl}$:

$$\varepsilon_{ij}^{dev,pl} = \sqrt{\left(\frac{\varepsilon_{ij}^{pl}-\varepsilon_{ij}^{pl,c}}{\|\varepsilon_{ij}^{pl}\|}\right)^2}.$$  \hspace{1cm} (1)

4. the volume average of accumulated shear strain on slip systems in decreasing order:

$$\gamma_{avg}^s = \langle \gamma_{ord}^{s,c} \rangle$$  \hspace{1cm} (2)

where $\gamma_{ord}^{s,c}$ is a vector of accumulated shear strain on slip systems in decreasing order for grain c.

5. the volume average of dislocation density:

$$\rho_{avg} = \langle \sum_s \rho^{s,c} \rangle$$  \hspace{1cm} (3)

where $\rho^{s,c}$ is a vector of dislocation density on slip systems for grain c.

6. crystal orientations, i.e. texture.

First, we compare the variation of selected quantities along the thickness direction after the CBT. The high variation in equivalent plastic strain over section points, shown in Fig 11a, is a result of different (plastic) strain histories experienced by section points. The top and the bottom point experience plastic strain path reversals, which add to the equivalent plastic strain, but subtract from the total plastic strain, causing a mismatch between the equivalent plastic strain and the axial plastic strain.
Fig. 11. Comparison of ST state at 0.172 axial plastic strain with CBT state after 4th cycle in terms of: (a) equivalent plastic strain, (b) macroscopic plastic strain, (c) deviation of grain plastic strain components, (d) volume average of accumulated shear strain on slip systems in decreasing order and (e) volume average of dislocation density.
component, $\varepsilon_{11}^{pl}$. On the other hand, the middle point does not experience the plastic strain path reversals and the equivalent plastic strain is not far from the current plastic strain in axial direction, Fig 11b. The average dislocation density, shown in Fig 11e, exhibits similar dependence with section points as the equivalent plastic strain. The plastic strain, the plastic strain deviation and the average shear strain on slip systems do not show appreciable change over section points in CBT, see Fig 11b-d. The comparison between the CBT and the ST is discussed next. The thickness plastic strain is lower for the CBT than for the ST, while the width strain is lower for the ST, see Fig 11b. More pronounced thinning in the CBT specimen compared to the ST specimen is likely coming from positive stress in width direction (stress component 22 shown in Fig 9b), preventing the contraction of the specimen in the width direction during tensile plastic deformation in axial direction. From Fig 11c it appears the plastic strain deviation for the ST is, for most part, above the plastic strain deviation for the CBT, suggesting a more uniform plastic deformation during the CBT process. The average accumulated shear strain on slip systems, shown in Fig 11d, is similar between the ST and the CBT. The average dislocation density for the CBT is slightly above the dislocation density for the ST, see Fig 11e.

Pole figures, showing the texture at 0.172 plastic strain for the ST and after 5.5 cycles for the CBT, are compared in Fig 12. The pole figures of the bottom, the middle and the top point through thickness for the CBT are similar in terms of the observed features and intensities. The ST pole figure has similar features as the CBT pole figures, while the intensities are higher for the ST. Apparently, the crystal reorientation is more rapid during the ST than during the CBT.
Fig. 11. Comparison of texture for (a) the ST at 0.172 axial plastic strain with (b) the CBT after 5.5 cycles having the same value of axial plastic strain.
5. Conclusions

The EPSC model material parameters were calibrated against experimental monotonic and cyclic stress-strain curves for AA6022-T4. The calibrated material model was used to define the material behavior for FE simulation of the CBT test in Abaqus. The simulated force-displacement and texture evolution during the CBT test match with the experimental measurements. During the CBT test, only regions in close vicinity of rollers experience plastic deformation. The regions close to the top and bottom surface of the specimen experience strain path reversals during the passage of rollers. Due to the asymmetric deformation conditions in the through thickness direction there is a gradient in the axial plastic strain, responsible for the presence of reaction bending moment at grips and characteristic unloaded shape of CBT specimens recorded in [5]. The comparison of the CBT deformation process and the ST, at the same level of axial plastic strain, shows that the two deformation processes result in similar material states with minor differences: (1) the plastic strain is more uniformly distributed over grains after the CBT process, (2) the dislocation density is slightly higher after the CBT processing, (3) the crystal rotation is happening at higher rate during the ST.

Acknowledgments

The FE model of CBT simulation was developed by Timothy Barrett. The CBT experimental data was collected and post-processed by Camille Poulin. The cyclic stress-strain response were provided by Toshihiko Kuwabara.

Appendix A

In this study, the backstress definition from [12, 17] was simplified by eliminating the interaction between slip systems. Removing the interaction between slip systems
helps the convergence by ensuring positive definiteness of matrices used in solution procedure i.e. hardening matrix [12].

The backstress evolution law defines the evolution of backstress on a slip system, $\tau_{bs}^{s}$, in function of shear strain on slip systems, $\gamma^s$. Elimination of latent hardening effects in the backstress evolution law is accomplished by constraining the backstress on a slip system, $\tau_{bs}^{s}$, to depend only on the shear strain on that slip system, $\gamma^s$. Closer examination of backstress evolution law from [17], shows that the slip system source of backstress fulfills the constraint for elimination of the latent hardening effects. Therefore, in this work we use the slip system source of backstress as the total backstress on a slip system. The evolution laws for $d\gamma^s > 0$ and $\tau_{bs}^{s+} > 0$ are:

$$\tau_{bs}^{s+} = \tau_{bs}^{sat}(1 - \exp(-\nu\gamma^s)),$$

(A1)

$$\tau_{bs}^{s-} = -A\tau_{bs}^{s+},$$

(A2)

where $\tau_{bs}^{sat}$ is a saturation value for the backstress, A is a parameter for asymmetric evolution of the backstress on a slip system in two different directions s+ and s-, $\gamma_b$ and $\nu$ are material parameters. The shear strain $\gamma^s$ is recorded from the point $\tau_{bs}^{s+} = 0$. The evolution laws for $d\gamma^s > 0$ and $\tau_{bs}^{s+} < 0$ are:

$$\tau_{bs}^{s+} = -(A + 1)\tau_{bs}^{sat} \exp\left(-\frac{\gamma^s}{\gamma_b}\right) + \tau_{bs}^{sat}$$

(A3)

$$\tau_{bs}^{s-} = -\frac{1}{A}\tau_{bs}^{s+}$$

(A4)

where the shear strain $\gamma^s$ is recorded from the point of local road reversal.
The definition of backstress with Eq. (A1-A4) ensures that the backstress matrix,

\[ h_{bs}^{ss'} = \frac{\partial \tau_{bs}^s}{\partial \gamma_{ss'}} \]

is diagonal, meaning it is a positive definite. Therefore, problems related to the loss of ellipticity of the tangent modulus are suppressed [12].

References


CHAPTER 7:

Summary and future work

In this work a multi-scale modeling framework for sheet metal forming simulations is developed. Finite element model of a forming process enforces the equilibrium at macro scale, while the elasto-plastic self-consistent model is used for scale transitioning from micro to macro scale and defining the constitutive behavior at macro scale. The elasto-plastic self-consistent model was coupled with finite element software Abaqus for 3D stress and shell elements. The continuum equations describing the elasto-plastic self-consistent modelling framework were integrated numerically with an implicit algorithm, facilitating use of large sub-steps in the integration procedure. As a result the computational efficiency of forming simulations is improved, while retaining the accuracy. By introducing concepts of reversible dislocations and backstress to the single crystal constitutive behavior, the elasto-plastic self-consistent model was further developed to accurately describe material behavior during strain path changes. Next, the developed model was calibrated against the experimentally measured mechanical response of aluminum alloy AA6022-T4. The calibrated model was used to simulate cup drawing process and predict the formed cup shape and springback. In addition, the model was utilized for simulation of the CBT test on AA6022-T4. The CBT test model results were validated with experimental measurements of force-displacement and texture evolution. The material state after the CBT test is similar to the material state after simple tension performed to the same level of plastic strain.

The developed modeling framework is general and can be used for metal forming simulations of other fcc and bcc and hcp materials. For instance, the CBT test on dual
phase steel can be simulated and compared with already available experimental measurements of mechanical response from [1]. In future, the predicted deformed cup shape can be validated against experimental measurements available from literature, for instance [2].

References
