Effective elastic properties of two-dimensional solids with inhomogeneities of irregular shapes

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EFFECTIVE ELASTIC PROPERTIES OF TWO-DIMENSIONAL SOLIDS WITH INHOMOGENEITIES OF IRREGULAR SHAPES

BY

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DISSERTATION

Submitted to the University of New Hampshire
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the Requirements for the Degree of

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in

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I dedicate this dissertation to my parents, and grandparents for their lifelong support, help and encouragement.
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ABSTRACT

EFFECTIVE ELASTIC PROPERTIES OF
TWO-DIMENSIONAL SOLIDS WITH INHOMOGENEITIES
OF IRREGULAR SHAPES

By

Jindrich Novak

University of New Hampshire, May, 2004

This work investigates the effective elastic properties of two-dimensional solids with inhomogeneities of various shapes. We develop a special procedure to evaluate the contribution of irregularly shaped inhomogeneities to these properties. The method can also be used to investigate the stress concentrations around the inhomogeneities. The procedure is based on the analysis of a representative volume element. We express the contribution of each inhomogeneity to the overall moduli of the composite in terms of the compliance contribution tensor. To calculate the components of this tensor, we devise a method that combines analytical and numerical approaches: Kolosov-Muskhelishvili complex variable technique and numerical conformal mapping. Application of this method to regularly shaped elastic inclusions, holes and rigid inclusions produces results that correspond well with the available analytical predictions. In the case of holes, the applicability of the finite element method is also investigated. The expressions for the effective elastic properties are first derived in the approximation of non-
interacting inhomogeneities. Then the results for interacting inhomogeneities incorporating the first order approximate schemes are presented.

To demonstrate the application of the method, we analyze a carbon fiber reinforced composite containing pores of irregular shapes. A two-step micromechanical procedure utilizing the concept of the compliance contribution tensor is used. We derive the closed form formulae for the contribution of fibers into the effective moduli and apply the procedure to determine the effective in-situ properties of pyrolytic carbon – a matrix phase formed during a densification process by chemical vapor infiltration.
CHAPTER I

INTRODUCTION

The concept of composite materials dates all the way back to antiquity. Mud bricks reinforced with straw were already used several centuries B.C. The history of the modern composites is however relatively new, with some of the major advancements made as recently as the end of the 20th century. Technological progress in many areas of science has enabled us to look at the micro and nano structure of the existing materials, create computerized models, design new materials with advanced mechanical, thermal and electronic properties, and manufacture them. Words such as lightweight, high-performance and smart have become synonyms for today’s composites. Thanks to their unique properties, they have become of high importance for nearly all branches of the industry, defense and space research, gradually replacing the conventional materials. The field continues to be very dynamic today. Nanoscience appears to be another step in the evolution of composite and smart materials, and new manufacturing methods are continuously being deployed as well.

In order to create more accurate models for simulating materials, scientists have to progress with their theoretical understanding of subject. Various approaches based on continuum mechanics have been successfully applied to describe material characteristics on the macro and microscale. While the reach of methods based on the analytical solutions is still limited, numerical techniques have become a great tool to model

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very complicated microstructures. They are, however, not universal. They require substantial computational power, and their accuracy has to be treated with caution. On the nanoscale, the continuum mechanics approach may not be appropriate and different methods, such as molecular dynamics, can be utilized.

1.1 Matrix-Based Composite Materials

This dissertation deals with the group of materials that are typically analyzed with the help of approaches based on continuum mechanics - matrix-based composites. Their characteristic feature is one continuous phase denoted as matrix. Other phases, commonly referred to as inhomogeneities, can be of various types. Inclusions are inhomogeneities formed from a material of different properties than those of the matrix. Note that in the notation of some other authors, for example Mura (1987), inclusion may represent a different object - a domain with the distribution of eigenstrains and eigenstresses. Holes, cavities or pores are empty spaces fully enclosed by the matrix material. In some cases, pores can be filled with a liquid phase (for example pores in salt water ice are filled with a highly saline fluid) or can be in direct contact with the inclusion. The microstructure of these materials may vary greatly. Typical examples are layered or unidirectional composites in which the matrix is reinforced by fibers packed in certain arrangements.

Matrix-based materials received a lot of attention from researchers in the second half of the twentieth century. Theoretical foundations have, however, been laid down even earlier. A generation of Russian scientists, including Kolosov G.V., Muskhelishvili N.I.,
Savin G.N., Sheremetiev M.P. etc., published numerous works on theoretical elasticity and plane boundary value problems in the first half of the last century. They were translated into English in the 1950's and 60's (Muskhelishvili, 1963 and Savin, 1961). Another significant contribution was Eshelby's (1957) solution to the problem of 3D elastic ellipsoidal inclusion embedded in infinite space. A substantial amount of literature on micromechanics of composites was published in the following decades by many scientists such as Hashin Z., Shtrikman S., Hill R., Budiansky B., Willis J.R., Walpole L.J., Milton G.W., all of whom contributed greatly to the field.

The approaches to analyze the material can be divided, in general, into two major categories. The first one, a direct solution for a given microstructure, puts emphasis on the geometry and orientation of inhomogeneities and tries to predict the behavior of a given composite. An alternative to dealing directly with the peculiarities of the microstructure is the construction of the upper and lower bounds (limiting values) on the effective properties, with or without some regards paid to the details of the microstructure. Hashin (1962, 1965) and Hashin and Shtrikman (1962, 1963) pioneered the basic idea of the bounds, soon followed by the works of Hill (1963, 1964), Walpole (1966, 1969), Kröner (1977), Willis (1977, 1981), Mura (1987), Avellaneda (1987), Milton and Kohn (1988), Torquato (2002) and others.
1.2 Direct Approach to the Effective Properties

Many approaches to the effective properties utilize the elasticity solutions for isolated inhomogeneities placed in infinite medium. The resulting estimates are then applicable to a variety of other microstructures exhibiting similar compositions of inhomogeneities' geometries. Other approaches try to solve the elasticity problem for the entire microstructure. In the latter case, except for a few special cases of the microstructure for which the analytical solutions are known (such as Hashin's (1962) composite spheres model, layered structures, coated ellipsoid assemblages, see Milton (2002) for the comprehensive overview of other microstructures), only direct numerical simulations are feasible. Their examples can be found in Day et al. (1992), Garboczi and Day (1995), Gusev (1997), Roberts and Garboczi (2000), Böhm et al. (2004), for example. These models tend to be very large and complex, especially in 3D, and considerable simplifications usually have to be introduced. Numerical results are generally not applicable to different microstructures.

Available analytical results in elasticity that can be utilized in the analysis of the effective properties of composites with holes and inclusions include various solutions of the Eshelby's problem (infinite body with a finite domain experiencing a distribution of eigenstrains or eigenstresses). Eshelby (1957) published his powerful solution for an ellipsoid. He observed that the ellipsoidal domain in the infinite space remotely loaded by a uniform strain exhibits constant distribution of stresses and strains. Mura et al. (1994) claimed that pentagonal star-shaped domains share this remarkable property as well. Contrary to Mura's conclusion, Rodin (1996) and Markenscoff (1997) proved that
polyhedral (polygonal in 2D) inclusion with such a property does not exist. Eshelby's problem for cuboid was studied by Faivre (1964), Sankaran and Laird (1976), Lee and Johnson (1977) and Chiu (1977). Mura (1987) gives the overview of the results for ellipsoid and cuboid. Various types of Eshelby's problems have been studied by many authors such as Seo and Mura (1979), Hu (1989), Yu and Sanday (1991) and others. Rodin (1996) gave the solution to the Eshelby's problem for polyhedron.

In 2D, one can utilize extensive work of Muskhelishvili (1963) and Savin (1961) on problems for holes and inclusions of regular shapes and, for example, Sheremetiev's (1949) approach to the hole reinforced by a regular elastic ring. Donnel (1941) first treated elastic inclusion of elliptical geometry embedded in a plate loaded by edge forces. Hardiman (1954) presented a complex variable solution for elastic elliptical inclusion placed in an infinite plane. He was also the first to notice that such inclusion exhibits uniform stress and strain fields under remotely applied tension. The problem of elliptical elastic inclusion was also investigated by Bhargava and Radhakrishna (1963) using energy method. Sendeckyj (1970) presented an elegant complex variable solution to elastic inclusions embedded in the infinite plane. His results for a general shape, however, require algebraic operations and are not suitable for numerical computations. Rodin (1996) published a solution to Eshelby's problem for polygons. Ru (1999) published solution to the Eshelby's problem for an infinite plane containing elastic inclusion of arbitrary shape. It requires, however, computation of the inverse map, which can be very troublesome, especially in the case of highly irregular geometries.

Works of these and other authors were extensively used in Kachanov et al. (1994) to obtain estimates of the effective properties of 2D composites (materials whose
microstructures can be modeled in two dimensions) with cavities and cracks of regular shapes. They were also used in Jasiuk (1995) for the case of composites with rigid inclusions of regular shapes. Solutions for the effective properties dealing with inhomogeneities of irregular shapes, however, are still scarce. For example, Nozaki and Taya (1997) presented results for the effective properties of a composite reinforced by arbitrarily shaped polygonal elastic fibers. Their work, however, contains a flaw discovered by Rodin (1998) and is applicable to the case of convex polygons only. Nozaki and Taya (2001) expanded their results to the effective properties of composites reinforced by convex polyhedral inclusions. Also, extensive literature on plane strain elastic properties of solids with circular elastic inclusions (a problem relevant to composites reinforced by unidirectional fibers of circular cross-section) is available; see for example Hashin and Rosen (1964), Hill (1964, 1965), Hashin (1972) and Ju and Zhang (1998). Closed form formulae for the ribbon-reinforced composites (modeled as elastic ellipsoidal cylinders) are presented in Zhao and Weng (1990). The motivation for the present work is to utilize the approach to the effective properties proposed by Kachanov et al. (1994) and devise an efficient method accurately accounting for 2D inhomogeneities of arbitrarily irregular geometries where no analytical solutions are available. General considerations and some results on micromechanical modeling of solids with heterogeneities can be found in books of Christensen (1979), Mura (1987), Aboudi (1991) and Nemat-Nasser and Hori (1993), Markov and Preziosi (2000), Milton (2002), Torquato (2002).

The Chapters of this dissertation are organized as follows: Chapter 2 introduces the basic concepts, describes the methodology of our micromechanical approach to the
effective elastic properties of composite materials with inhomogeneities and gives an overview of the related results obtained by other scientists. Chapter 3 presents an effective numerical method to solve the elasticity problems for 2D irregularly shaped inhomogeneities placed in the infinite plane. Examples of the elastic fields are presented for the cases of various elastic inclusions as well as for the limiting cases of holes and rigid inclusions. The Chapter also shows the application of the finite element method to the cases of holes and utilizes both numerical methods to obtain the hole's compressibility. Comparisons with available analytical solutions are also provided. Chapter 4 presents formulae for the effective properties of various microstructures and shows some results for the materials with various combinations of inhomogeneities. In Chapter 5, we apply the methodology to analyze carbon/carbon composite material densified by the chemical vapor infiltration. This Chapter first studies the microstructure and describes the micromechanical analysis. Then, with the help of the relations provided in Chapter 4, it accounts for the contributions of the composite's constituents and describes the procedure to determine the unknown effective in-situ mechanical properties of the matrix phase. Images of the microstructure and various information presented in Chapter 5 have been obtained in collaboration with the Institute of Solid Mechanics at the University of Karlsruhe, Germany.
CHAPTER II

COMPLIANCE CONTRIBUTION TENSOR APPROACH TO EFFECTIVE ELASTIC PROPERTIES OF SOLIDS WITH INHOMOGENEITIES

This Chapter describes a general micromechanical approach to obtain the effective properties of matrix-based heterogeneous materials. Using this approach, the contribution of all defects and inhomogeneities is accounted for through the compliance contribution tensor $\mathbf{H}$. The Chapter introduces this tensor, outlines the procedure to derive its components and show its use in various micromechanical modeling schemes.

2.1 Representative Volume Element

The procedure presented in this work is based on the concept of a representative volume element RVE (representative area element RAE in 2D) traditionally utilized by researches in micromechanical modeling of composite materials. By its definition, RVE statistically represents the microstructure of a heterogeneous material, and therefore we assume that its behavior and mechanical properties are identical to those of that material. We substitute this heterogeneous RVE with an equivalent
homogeneous material, i.e. having the same overall properties as the composite (Fig. 2.1). Literature often refers to this as homogenization; see, for example, Nemat-Nasser and Hori (1993) or Mura (1987).

\[
\begin{align*}
\mathbf{\varepsilon} &= \mathbf{S}_M : \mathbf{\sigma} + \text{influence of inhomogeneities} \\
\mathbf{\varepsilon} &= \mathbf{S} : \mathbf{\sigma}
\end{align*}
\]

Fig. 2.1 Homogenization of heterogeneous material. \( \mathbf{S}_M \) and \( \mathbf{S} \) are the compliance tensors of matrix and effective material, respectively.

The goal of the procedure is to find the effective elastic compliance tensor \( \mathbf{S} \) that relates the values of macroscopic strain and stress tensors, \( \mathbf{\varepsilon} \) and \( \mathbf{\sigma} \), as

\[
\mathbf{\varepsilon} = \mathbf{S} : \mathbf{\sigma},
\]

where colon denotes contraction over two indices. Macroscopic strain \( \mathbf{\varepsilon} \) and stress \( \mathbf{\sigma} \) are defined with the help of the divergence theorem in 2D case (footnote of Hill, 1963) as

\[
\begin{align*}
\mathbf{\varepsilon} &= \frac{1}{2A} \int (\mathbf{u n} + \mathbf{n u}) \, dy, \\
\mathbf{\sigma} &= \frac{1}{A} \int \mathbf{t x} \, dy,
\end{align*}
\]

(2.2)
In the Eqs. (2.2), $A$ is the representative area element (RAE) with boundary $\gamma$ and $u$, $n$, $t$ and $x$ are the displacement, outward unit normal, traction and position vectors of the boundary points, respectively, see Fig. 2.2. Expressions $un$, $nu$ and $tx$ are the dyadic products of the corresponding vectors.

![Fig. 2.2 Representative area element](image)

To characterize the contribution of inclusions and holes into the effective elastic compliance, we introduce the inclusion compliance contribution tensor $H^{\text{RAE}}$ as

$$S=S_M + H^{\text{RAE}},$$

(2.3)

where $S_M$ is the compliance tensor of matrix material. The compliance contribution tensor ($H$-tensor) has been used by Kachanov et al. (1994) and Tsukrov and Novak (2002) to analyze solids with various 2D and 3D holes, and by Sevostianov and

### 2.2 Compliance Contribution Tensor (H-tensor) of Inclusion

The procedure is based on the results for one inclusion. First, let us investigate the contribution of the inclusion into the effective compliance. We represent the total strain and stress tensors (as defined by Eqs. (2.2)) in a reference area \( \bar{A} \) containing an inclusion of area \( A_i \) (Fig. 2.3) as sums

\[
\varepsilon = \varepsilon_M + \Delta \varepsilon, \quad \sigma = \sigma_M + \Delta \sigma, \quad (2.4)
\]

where

\[
\varepsilon_M = \frac{1}{A} \int_A \varepsilon(x) dA, \quad \sigma_M = \frac{1}{A} \int_A \sigma(x) dA, \quad (2.5)
\]

are related to the average strain and stress in the matrix as \( \varepsilon_M = \frac{A_M}{A} (\varepsilon)_M \) and \( \sigma_M = \frac{A_M}{A} (\sigma)_M \).
Inclusion contributions $\Delta \varepsilon$ and $\Delta \sigma$ are derived from the divergence theorem as:

$$
\Delta \varepsilon = -\frac{1}{2A} \int (un + nu) d\Gamma, \quad \Delta \sigma = -\frac{1}{A} \int t x d\Gamma, 
$$

(2.6)

where $n$ is the unit normal to inclusion boundary $\Gamma$ directed inward the inclusion.

Then, the contribution of the inclusion to the overall compliance of $\tilde{A}$ is given by tensor $H$, and the following relation must hold

$$
H : \sigma = \Delta \varepsilon - S_M : \Delta \sigma.
$$

(2.7)

Expression (2.7) is obtained by substituting Eqs. (2.3) and (2.4) into Eq. (2.1).
With the help of Eqs. (2.6), (2.7) and using the expression for the area of an inclusion
\[ A_i = \frac{1}{2} \int \left( x_1 \frac{dx_2}{d\Gamma} - x_2 \frac{dx_1}{d\Gamma} \right) d\Gamma, \]
we can also introduce tensor \( H^* = \frac{\tilde{A}}{A_i} H \). This tensor is used in Chapter 4 in the expressions for the effective properties.

Tensor \( H \) possesses the usual symmetries of the elastic compliance tensor \( (H_{ijkl} = H_{jilk} = H_{klij}) \) and, in 2D case, has no more than six independent components.

In the local coordinate system \( x_1x_2 \) with unit vectors \( e_1 \) and \( e_2 \) (Fig. 2.3), the inclusion compliance contribution tensor for an arbitrary 2D inclusion has the following structure

\[
H = H_{1111} e_1 e_1 e_1 e_1 + H_{2222} e_2 e_2 e_2 e_2 + H_{1122} (e_1 e_1 e_1 e_2 + e_2 e_2 e_1 e_1) + \\
+ H_{1211} (e_1 e_2 e_1 e_1 + e_2 e_1 e_1 e_2 + e_1 e_1 e_2 e_1 + e_2 e_2 e_1 e_1) + \\
+ H_{1222} (e_1 e_2 e_2 e_1 + e_2 e_1 e_1 e_2 + e_1 e_1 e_2 e_2 + e_2 e_2 e_1 e_2) + \\
+ H_{1212} (e_1 e_2 e_1 e_2 + e_1 e_2 e_2 e_1 + e_2 e_1 e_2 e_1 + e_2 e_2 e_1 e_2) \\
(2.8)
\]

If the shape of the inclusion has some geometric symmetries, the number of independent components of \( H \)-tensor is reduced (see Appendix A). For example, for the shapes with two perpendicular axes of symmetry the number of independent constants reduces to four since

\[
H_{1222} = H_{1211} = 0 \quad (2.9)
\]

In the case of shapes that are symmetrical with respect to 90 degree rotation (objects that superimpose upon themselves after every 90 degree rotation; for example, square), the number of independent coefficients reduces to three since
Finally, for the shapes that are symmetrical with respect to the rotation other than 90 and 180 degrees (for example equilateral triangles) the following relationship holds:

\[ H_{\overline{1}11_1} = H_{222_2} \]  

(2.10)

and the number of independent constants reduces to two (Tsukrov et al., 2003). As discussed in Kachanov et al. (1994), an isotropic plate with any orientational distribution of such defects exhibits overall isotropic behavior. In the text to follow, these shapes are called isotropic.

To find the components of \( \mathbf{H} \)-tensor for a particular shape, we assume that the total stress, Eq. (2.4), in the reference area \( \tilde{A} \), is equal to the applied remote stress, and evaluate the additional strain and stress tensors given by Eqs. (2.6). Let us consider a remotely applied uniaxial tension \( P \) inclined at an angle \( \theta \) to \( x_1 \)-axis as shown in Fig. 2.4.
The stress tensor for such loading is

\[
\sigma = P \left[ \cos^2 \theta \mathbf{e}_1 \mathbf{e}_1 + \sin^2 \theta \mathbf{e}_2 \mathbf{e}_2 + \sin \theta \cos \theta (\mathbf{e}_1 \mathbf{e}_1 + \mathbf{e}_2 \mathbf{e}_2) \right].
\] (2.12)

Contraction of this tensor with \( \mathbf{H} \) given by Eq. (2.8) produces the following expressions:

\[
(\mathbf{H} : \sigma)_{11} = \frac{P}{2} \left[ (H_{1111} + H_{1122}) + (H_{1111} - H_{1122}) \cos 2\theta + 2H_{1211} \sin 2\theta \right]
\]

\[
(\mathbf{H} : \sigma)_{22} = \frac{P}{2} \left[ (H_{2222} + H_{1122}) - (H_{2222} - H_{1122}) \cos 2\theta + 2H_{1222} \sin 2\theta \right]
\] (2.13)

\[
(\mathbf{H} : \sigma)_{12} = \frac{P}{2} \left[ (H_{1211} + H_{1222}) + (H_{1211} - H_{1222}) \cos 2\theta + 2H_{1212} \sin 2\theta \right]
\]
Now, the components of $H$ are obtained from Eq. (2.7) by comparing these expressions with the corresponding elasticity predictions for additional strain and stress given by Eqs. (2.6) for various values of angle $\theta$.

### 2.3 Micromechanical Models of Solids with Inclusions

$H$-tensors for inclusions of various geometries can be utilized to predict the effective elastic moduli using either non-interaction approximation or some first-order micromechanical modeling schemes. In the approximation of non-interacting inclusions, it is assumed for each inclusion that the reference area $\tilde{A}$ is equal to RAE, and the stress field is not disturbed by the presence of other inclusions. Then, the overall response of the material with many non-interacting inclusions can be characterized as

$$S = S_M + H^{NI},$$

(2.14)

where tensor $H^{NI}$, the non-interaction approximation of tensor $H^{RAE}$, is a sum of the contributions of all the inclusions in RAE

$$H^{NI} = \sum H^{(k)}$$

(2.15)

(summation may be replaced by integration over orientations, if computationally convenient). Non-interaction approximation is only applicable, however, for small inclusion concentrations when interaction effects can be neglected.
The predictions of more advanced approximate micromechanical schemes are obtained from $H^N$. Detailed discussion of the structure of $H$-tensors in different approximate schemes can be found in Tsukrov et al. (2003). According to the authors, in the case of Mori-Tanaka approximation (Mori and Tanaka (1973), Benveniste (1987)), when each inclusion is assumed to be subjected to the remote stress equal to the average stress in the matrix phase, compliance contribution tensor $H^{MT}$ and the effective compliance $S$ are derived as functions of the inclusion volume fraction $f$ as

$$H^{MT} = H^N : \left[ \left(1 - f\right) \left(S_i - S_M\right) + H^N \right]^{-1} : \left( S_i - S_M \right), \quad S = S_M + H^{MT} \quad (2.16)$$

Self-consistent method (for example see Hill (1965) and Budiansky (1965)), that assumes the inclusions to be placed in the equivalent matrix having the overall property of composite $S$, approximates $H$ tensor and the effective compliance as

$$H^{SC} = \left( S_i - S_M \right) \cdot \left( S_i - S \right)^{-1} H^N \left( S, S_i \right), \quad S = S_M + H^{SC} \quad (2.17)$$

where $H^N(S, S_i)$ is the non-interaction compliance tensor when inclusion $S_i$ is placed into matrix $S$. A much improved form of this approximate scheme is generalized self-consistent method (Huang and Hu, 1995 and Jiang et al., 2003), that assumes the inclusion to be placed in a finite matrix, which is embedded into an infinite composite of yet unknown effective moduli. In the differential method (McLaughlin, 1977), the inclusions are incrementally added to the material until the final inclusion volume
fraction \( f \) is reached. To obtain the estimates of \(\mathbf{H}\) tensor and effective compliance, the differential equation in (2.18) must be solved.

\[
\frac{d\mathbf{H}^{\text{DIFF}}}{dt} = \frac{1}{f(1-f)} \mathbf{H}^{\text{NI}}(\mathbf{S}(t), \mathbf{S}_i),
\]

\[
\mathbf{S} = \mathbf{S}_M + \mathbf{H}^{\text{DIFF}} \tag{2.18}
\]

where \(\mathbf{S}(t)\) denotes the compliance of composite having inclusion volume fraction \( t \) and Eq. (2.18) is solved with the initial condition \( \mathbf{H}^{\text{DIFF}}(t = 0) = 0 \).

Dvorak and Srinivas (1999) proved that the following assumption leads to the variety of approximate schemes that can be utilized to obtain the effective properties: having RVE subjected to the displacement field \( \mathbf{u} = \mathbf{e}^0 \cdot \mathbf{x} \), the average strain in all the inclusions is the same as the average strain in the inclusion placed in some comparison medium subjected to the uniform far field strain \( \mathbf{e}^0 \). Tsukrov et al. (2003) have shown that the approximations of \(\mathbf{H}\) tensor and the effective compliance are obtained in this case from

\[
\mathbf{H}^{\text{DS}} = (\mathbf{S}_i - \mathbf{S}_M)(\mathbf{S}_i - \mathbf{S}^*)^{-1} : \mathbf{H}^{\text{NI}}(\mathbf{S}^*, \mathbf{S}_i),
\]

\[
\mathbf{S} = \mathbf{S}_M + \mathbf{H}^{\text{DS}} \tag{2.19}
\]

where \(\mathbf{S}^*\) is the compliance tensor of the comparison medium. Different choices of the comparison medium yield various predictions. Dvorak and Srinivas (1999) have also shown that the Mori-Tanaka and self-consistent schemes, described by Eqs. (2.16) and (2.17), can be mathematically treated in the same fashion with only a different choice of the comparison medium. These authors have also observed that the Mori-Tanaka scheme,
Eq. (2.16), represents the lower (upper) bound on the effective moduli when the stiffness of the inclusions is lower (higher) than the one of a matrix material.

Thus, the effective elastic properties of composites with irregularly shaped inclusions can be expressed in terms of tensor $H$. To find $H$ for each inclusion's geometry, the additional strain and stress tensors must be calculated and substituted into Eq. (2.7). This is done by solving the elasticity problem for one inclusion and utilizing Eqs. (2.6). In the case of some regular shapes, the elasticity problem can be solved analytically (for example Hardiman's (1954) solution for ellipse), and the explicit expressions for additional strain and stress can be found. The following Chapter describes an effective numerical technique for solving the elasticity problem for irregularly shaped inclusions under remotely applied stress and uses its results to obtain the components of $H$ tensor for selected examples of inclusions and holes.
This Chapter presents a numerical conformal mapping (NCM) procedure used to analyze the stress and displacement fields in and around irregularly shaped inclusions or holes, placed in an infinite plane subjected to remotely applied loading. The procedure is utilized in Sections 3.3 to determine the components of the compliance contribution tensor $\mathbf{H}$, introduced in Chapter 2, in the cases of elastic and rigid inclusions. Section 4 employs both the NCM and finite element method to analyze holes and investigates their compressibility. The predictions of both numerical methods, and analytical results (where available) are compared.

3.1 Numerical Conformal Mapping Method

The numerical technique presented here solves the elasticity problem for a 2D inclusion of arbitrary shape placed in the infinite plane and subjected to remotely applied uniform tension (Fig. 2.3). (Note that in 2D elasticity any stress state can be represented as a sum of two tensions/compressions in principal directions.) The procedure is based on the complex variable approach; see, for example, Muskhelishvili (1963) and Savin 1961). It uses the conformal mapping of the exterior of an inclusion onto the interior of a unit
circle with the mapping function found by numerical evaluation of the Schwarz-Christoffel integral. Application of this numerical conformal mapping method to the analysis of irregularly shaped holes in elastic matrix is described in Tsukrov and Novak (2000, 2002).

Note that Hardiman (1954) gave the analytical solution to the elasticity problem for an elliptical inclusion in the infinite plane. For polygonal shapes, one can use the components of the Eshelby's tensor provided by Rodin (1996); see also Nozaki and Taya (1997, 2001) and Rodin (1998). A complex variable approach to the Eshelby's problem is also presented in Ru (1999). Greengard and Helsing (1998) proposed an efficient numerical algorithm to solve the Sherman integral equation (Sherman, 1959), and applied it to analyze solids with periodic arrangements of irregularly shaped inclusions. The method is, however, applicable only to two material configurations and is not valid for holes (Crouch and Mogilevskaya, 2003). A similar approach was used in Helsing and Johnson (2001, 2002) to analyze plates perforated with holes. Our method solves the elasticity problem for an arbitrarily shaped elastic inclusion placed in infinite plane loaded by uniaxial tension at infinity. The method is also applicable to the limiting cases of holes and rigid inclusions.

Let us consider an inclusion of arbitrary shape in the complex plane $z = x_1 + ix_2$ with the origin inside of the inclusion (Fig. 2.3). The solution requires mapping of the interior of the unit circle in canonical plane $\zeta$ onto the exterior of the inclusion region in $z$ plane by the analytical mapping function $\omega(\zeta)$. It is well-known that for the case of polygons this can be done by evaluation of the Schwarz-Christoffel integral.
\[ \omega(\zeta) = \prod_{k=1}^{n} \left(1 - \frac{\zeta}{\zeta_k}\right)^{1-\beta_k} \frac{1}{\zeta^{\gamma}} d\zeta, \]  

(3.1)

where \( \beta_k \pi \) are the interior angles of the polygon and \( \zeta_k \) are the prevertices (points on the unit circle in the canonical plane that correspond to the vertices of the polygon \( z_k \)).

To obtain a conformal mapping function \( \omega(\zeta) \) for an arbitrarily shaped inclusion, we first approximate the boundary of the inclusion by an \( N \)-sided polygon with vertices on the boundary of the inclusion (Fig. 3.1).

Fig. 3.1 NCM for the inclusion of irregular shape: points on the boundary of the circle correspond to the vertices of the approximating polygon

The accuracy of this approximation depends entirely on the number of vertices. While in the case of regular polygons the Schwarz-Christoffel integral in Eq. (3.1) can be evaluated analytically (Savin, 1961), for more complicated shapes this integral has to be evaluated numerically. Our procedure utilizes Matlab Schwarz-Christoffel toolbox developed by Driscoll (1996).

While the numerical evaluation of the mapping function (3.1) using Driscoll's program is very accurate, calculation of its derivatives tends to degenerate and become very
inaccurate close to the singular points: origin $\zeta = 0$ and prevertices $\zeta_k$. Tsukrov and Novak (2002) attempted to rectify the problem for the case of holes by recalculating the map at evenly spaced points in the canonical domain on the unit disc. As a result, sharpest regions of the original approximating polygon were eliminated, causing further deviation from the original shape.

Present solution tries to avoid sharp corners of the approximating polygon and eliminate the inaccuracy in calculations of the derivatives. The mapping function is obtained in its closed form for the shape closely resembling the original approximating polygon. The procedure is described in the next paragraph.

The integrand in (3.1) is expanded in truncated Laurent series with the center at the origin $\zeta = 0$

$$\prod_k \left(1 - \frac{\zeta}{\zeta_k}\right)^{1-\delta_k} \frac{1}{\zeta^2} \approx \sum_{j=-2}^{\infty} a_j \zeta^j$$

The integrand in Eq. (3.1) is analytic and single valued in the entire domain of the unit disk except at singular points: prevertices $\zeta = \zeta_k$ and the origin $\zeta = 0$. To ensure the single valuedness of the resulting map coefficient $a_{-1} = 0$. Series (3.2) is convergent in the entire domain of the unit disk except at the specified singular points on the boundary and the origin. The accuracy of this approximation depends on the number of terms $M$ in the expansion. Fig. 3.2 illustrates this procedure on a rather complicated original inclusion shape.
As can be seen, only 15 terms of the expansion are used to achieve relatively good correspondence of the geometries. Integrating (3.1) with the integrand approximated by series (3.2) gives accurate values of the mapping function. Its derivatives are then obtained by direct differentiation of series (3.2).

Having constructed the mapping function $\omega(z)$, we are able to utilize the Kolosov-Muskhetishvili approach to solve the elasticity problem for a 2D inclusion in an infinite plane loaded by remotely applied uniform tension $P$ (Fig. 2.4). According to this approach (Muskhelishvili, 1963), the displacements $u$, $v$ and stresses $\sigma_{xx}$, $\sigma_{yy}$ and $\tau_{xy}$ in the plate and inclusion can be expressed in terms of four analytical functions of complex variables (stress functions, or complex potentials) $\varphi_M(z)$, $\psi_M(z)$, $\varphi_I(z)$ and $\psi_I(z)$ as
\[ u^M + iv^M = \frac{3 - \nu_M}{E_M} \varphi(\zeta) - \frac{1 + \nu_M}{E_M} \left[ \frac{\omega(\zeta)}{\omega'(\zeta)} \varphi'_M(\zeta) + \psi'_M(\zeta) \right], \]

\[ \sigma_{xx}^M + \sigma_{yy}^M = 4 \text{Re} \frac{\varphi'_M(\zeta)}{\omega'(\zeta)}, \]

\[ \sigma_{yy}^M - \sigma_{xx}^M + 2i \tau_{xy}^M = 2 \left[ \frac{\varphi''_M(\zeta)}{\omega''(\zeta)} - \frac{\varphi'_M(\zeta)}{\omega'(\zeta)} \frac{\omega''(\zeta)}{\omega'(\zeta)} + \frac{\psi'_M(\zeta)}{\omega'(\zeta)} \right], \quad (3.3) \]

\[ u' + iv' = \frac{3 - \nu_I}{E_I} \varphi_I(z) - \frac{1 + \nu_I}{E_I} \left[ z \varphi'_I(z) + \psi'_I(z) \right], \]

\[ \sigma'_{xx} + \sigma'_{yy} = 4 \text{Re} \varphi'_I(z), \]

\[ \sigma'_{yy} - \sigma'_{xx} + 2i \tau'_{xy} = 2 \left[ z \varphi''_I(z) + \psi''_I(z) \right], \]

where \( E_M, \nu_M \) and \( E_I, \nu_I \) are the Young's moduli and Poisson's ratios of the matrix and inclusion materials in the case of plane stress. In the case of plane strain, the expressions \( E = E/(1 - \nu^2) \) and \( \nu = \nu/(1 - \nu) \) must be substituted for \( E \) and \( \nu \).

The stress functions for the infinite region of the matrix can be generally expressed as (Muskhelishvili 1963, Savin 1961):

\[ \varphi_M(\zeta) = \frac{X + iY}{2\pi \left( 1 + \frac{3 - \nu_M}{1 + \nu_M} \right)} \ln(\zeta) + (B_1 + iC_1) \omega(\zeta) + \sum_{n=0}^{\infty} \alpha_n^M \zeta^n, \]

\[ \psi_M(\zeta) = -\frac{3 - \nu_M}{1 + \nu_M} \frac{(X - iY)}{2\pi \left( 1 + \frac{3 - \nu_M}{1 + \nu_M} \right)} \ln(\zeta) + (B_2 + iC_2) \omega(\zeta) + \sum_{n=0}^{\infty} \beta_n^M \zeta^n, \]

where \( X + iY \) is the external force vector acting on the boundary, \( B_1, C_1, B_2, C_2, \alpha_n^M \)

and \( \beta_n^M \) are unknown constants. Since no external forces are applied to the boundary, one
may set $X = Y = 0$. Constant $C_1$ can be related to the rotation of the infinitely distant part of the plane $e_m$ (Muskhelishvili 1963) as

$$C_1 = \frac{2G_M e_m}{1 + 3 - \nu_M},$$

(3.5)

As this constant does not alter the stress distribution and displacements (except rigid body rotation), it remains indeterminate. To restrict the rigid body rotation of infinitely distant parts of the plane to zero one must set $C_1 = 0$. It is also known that constants $B_1, B_2$, and $C_2$ express the state of stress at infinity (Muskhelishvili, 1963 and Savin, 1961). For a plate loaded by remote uniaxial tension $P$ at angle $\theta$ from $x_1$-axis (Fig. 2.4), these constants take values $B_1 = P/4, B_2 = (P/2)\cos 2\theta$ and $C_2 = (P/2)\sin 2\theta$.

The results of the previous paragraph suggest that the representations of the stress functions in Eq. (3.4) can be recast in the following form:

$$\varphi_M(\zeta) = \varphi_{M,1}(\zeta) + \varphi_{M,0}(\zeta), \quad \psi_M(\zeta) = \psi_{M,1}(\zeta) + \psi_{M,0}(\zeta),$$

(3.6)

where $\varphi_{M,1}(\zeta) = (P/4)\omega(\zeta)$ and $\psi_{M,1}(\zeta) = -(P/2)e^{-2i\theta}\omega(\zeta)$ are the stress functions for the plate without inclusion (Savin, 1961). The additional terms, $\varphi_{M,0}(\zeta)$ and $\psi_{M,0}(\zeta)$, correspond to the disturbance in the stress field caused by the presence of inclusion and are expressed in the form of Taylor series.
\[ \varphi_{M,0}(\zeta) = \sum_{n=0}^{\infty} \alpha_n^M \zeta^n, \quad \psi_{M,0}(\zeta) = \sum_{n=0}^{\infty} \beta_n^M \zeta^n. \quad (3.7) \]

So far unknown coefficients \( \alpha_n^M \) and \( \beta_n^M \) have to be determined from the displacement and stress continuity conditions across the interface.

To ensure proper behavior of displacements and stresses at infinity, caused by the disturbance fields due to the presence of the inclusion, functions (3.7) have to be investigated as \( \zeta \to 0 \), or correspondingly \( z \to \infty \). With the help of Eqs. (3.3) we have

\[
\lim_{\zeta \to 0} \left( u_o^M + i v_o^M \right) = \lim_{\zeta \to 0} \left\{ \frac{3 - \nu^M}{E^M} \varphi_{M,0}(\zeta) - \frac{1 + \nu^M}{E^M} \left[ \frac{\omega(\zeta)}{\omega'(\zeta)} \varphi'_{M,0}(\zeta) + \psi_{M,0}(\zeta) \right] \right\} = \frac{1 + \nu^M}{E^M} \left( \frac{3 - \nu^M}{1 + \nu^M} \alpha_0^M - \beta_0^M \right)
\]

\[
\lim_{\zeta \to 0} \left( \sigma_{xx,0}^M + \sigma_{yy,0}^M \right) = \lim_{\zeta \to 0} \left\{ 4 \text{Re} \frac{\varphi'_{M,0}(\zeta)}{\omega'(\zeta)} \right\} = 0
\]

\[
\lim_{\zeta \to 0} \left( \sigma_{yy,0}^M - \sigma_{xx,0}^M + 2i \tau_{xy,0}^M \right) = \lim_{\zeta \to 0} \left\{ 2 \left[ \frac{\varphi_{M,0}(\zeta)}{\omega^2(\zeta)} - \varphi'_{M,0}(\zeta) \frac{\omega''(\zeta)}{\omega'^2(\zeta)} \right] \frac{\omega(\zeta)}{\omega'(\zeta)} \right\} = 0
\]

Expressions in Eq. (3.8) are evaluated in Appendix C. It can be seen that disturbance stresses and displacements at infinity remain bounded. The terms involving constants \( \alpha_0^M \) and \( \beta_0^M \) reflect pure rigid body translation of the infinitely distant parts of the plate. As these constants do not alter the state of stress and remain always undetermined, one can restrict the displacements of the infinitely distant parts of the plate to zero, i.e.
Muskhelishvili (1963), who arrives to this condition in a somewhat different way, shows that it also ensures the uniqueness of functions \( \phi_{M,0}(\zeta) \) and \( \psi_{M,0}(\zeta) \) in Eqs. (3.6) and (3.7). Thus, both displacements and stresses are bounded at infinity and all the functions for the matrix region are fully determinable.

It should be noted that while stresses at infinity caused by the functions \( \phi_{M,1}(\zeta) \) and \( \psi_{M,1}(\zeta) \) in Eq. (3.6) remain bounded and express the uniaxial tension \( P \), the associated displacements remain unbounded. This fact, however, has no influence on the calculations.

The stress functions for the inclusion region, \( \phi_i(z) \) and \( \psi_i(z) \), are expanded in series of Faber polynomials \( P_n(z) \) that are characteristic for the given domain (Smirnov and Lebedev, 1968) and must be computed beforehand. (We used the Matlab Schwarz-Christoffel toolbox developed by Driscoll, 1996.)

\[
\phi_i(z) = \sum_{n=1}^{\infty} \alpha_n^i P_n(z), \quad \psi_i(z) = \sum_{n=1}^{\infty} \beta_n^i P_n(z). \tag{3.10}
\]

Some discussion on the usage of Faber polynomials in the problems of two-dimensional elasticity can be found in Levin and Zingerman (2002).

To ensure that the functions are fully determinable, conditions analogous to (3.9) must also be satisfied by the stress potentials (3.10) in the inclusion region. As a result, two
constants from each region related to the rigid body motion of the entire system remain arbitrary and have to be selected to make the problem fully determinable. Setting \( \alpha_0^M = \beta_0^M = 0 \) yields functions (3.7) in the following final form:

\[
\varphi_{M,0}(\zeta) = \sum_{n=1}^{\infty} \alpha_n^M \zeta^n, \quad \psi_{M,0}(\zeta) = \sum_{n=1}^{\infty} \beta_n^M \zeta^n.
\] (3.11)

The coefficients in series (3.10) and (3.11) are calculated from the conditions satisfying the continuity of the displacements and boundary force resultants across the interface between the inclusion and matrix, i.e.

\[
(u + iv)^l = (u + iv)^M, \quad (f_1 - if_2)^l = (f_1 - if_2)^M.
\] (3.12)

Substitution of Eqs. (3.3) and (3.6) into the first equation of (3.12) yields the following form of the displacement continuity condition:

\[
- \frac{P(1 + \nu_M)}{E_M} \left[ \frac{\omega(\zeta)}{4} \left( \frac{3 - \nu_M}{1 + \nu_M} - 1 \right) + \frac{e^{2i\theta}}{2} \frac{\omega(\zeta)}{\phi(\zeta)} \right] = \frac{3 - \nu_M}{E_M} \phi(\zeta)
\]

\[
- \frac{1 + \nu_M}{E_M} \left[ \frac{\omega(\zeta)}{\omega'(\zeta)} \phi'(\zeta) + \psi'(\zeta) \right] + \frac{1 + \nu_L}{E_L} \left[ \frac{\omega(\zeta)}{\omega'(\zeta)} \phi'(\zeta) + \psi'(\zeta) \right] - \frac{3 - \nu_L}{E_L} \phi(z)
\] (3.13a)
The force resultant boundary condition takes the form:

\[
-\frac{P}{2} \left[ \phi(\xi) - e^{2i\theta} \phi'_{\alpha}(\xi) \right] = \phi_{M,\alpha}(\xi) + \frac{\phi(\xi)}{\phi'_{M,\alpha}(\xi)} \psi_{M,\alpha}(\xi) + \psi_{M,\alpha}'(z) - z \psi_{M,\alpha}'(z) - \psi_{M,\alpha}'(z)
\]

(3.13b)

By requesting that Eqs. 3.13a,b are satisfied at a discrete set of boundary points, we obtain a system of linear equations for unknown coefficients \(\alpha^M_n, \beta^M_n, \alpha^I_n,\) and \(\beta^I_n\). After this system is solved, the stresses and displacements in both domains and on inclusion boundary can be readily obtained from Eqs. (3.3). With the above procedure, 60-150 boundary points proved to be sufficient to obtain very accurate results for most of the tested shapes. The obtained boundary displacements and tractions can be used to calculate the components of additional strain and stress tensors, as shown in Section 3.3.

### 3.2 Elastic Fields Around Inclusions

#### 3.2.1 Stresses Around and Within Elastic Inclusions

Figs. 3.3 - 3.5 illustrate the distribution of stress fields for elastic inclusions of elliptical (of eccentricity 2.5:1) and arbitrary shape obtained using the NCM technique presented in the previous section. The inclusions are embedded into an infinite plane loaded by a remote uniaxial tension \(P = 1 Pa\) inclined at angle \(\theta = -45^\circ\) to \(x_1\) axis (see Fig. 3.6). The material properties are \(E_M = 10000 Pa, \ E_I = 100000 Pa, \ \nu_M = 0.25\) and \(\nu_I = 0.05\).
As first observed by Hardiman (1954), elliptical region within an infinite plane loaded by a remotely applied uniaxial tension exhibits constant distribution of stresses. In 3D, this phenomenon was first observed and proven by Eshelby (1957). As of today (to the knowledge of the author) no other scientist has provided proof that a different geometry shares this remarkable property of the ellipsoidal domain. As expected, numerically calculated results in Fig. 3.3 show constant distribution of stresses within elliptical inclusion. Also, due to higher local curvature of the boundary, the irregular inclusion experiences higher stress concentrations than elliptical inclusion.
Fig. 3.3 Elastic stress fields in the vicinity and within elastic inclusions of elliptical and irregular shapes.
The deformed shape of these elastic inclusions can be seen in Fig. 3.6, along with hypotrochoidal triangular inclusion of the same material properties. The deformed configurations are given in a magnification of 60000:1. The boundaries of these inclusions were discretized using 40 (elliptical) to 150 (irregularly shaped inclusion) points.
Fig. 3.6 Deformation of elastic inclusions under uniaxial tension. The boundaries with points represent the undeformed configurations.
(a) ellipse of eccentricity 2.5:1, (b) triangular hypotrochoid, (c) irregularly shaped inclusion
For illustration, Fig. 3.7 also presents the deformed shapes of selected irregular elastic inclusions (with the material properties $E_I = 100000 Pa$, $E_M = 10000 Pa$, $\nu_I = 0.05$ and $\nu_M = 0.25$). Their boundaries were discretized using 100 points in both cases. The deformed configurations are given in a magnification of 60000:1.

Fig. 3.7 Deformation of irregular elastic inclusions under uniaxial tension. The boundaries with points represent the undeformed configurations.
3.2.2 Stresses Around Rigid Inclusions

The NCM procedure described in Section 3.1 can be effectively applied to determine the elastic fields and compliance contribution tensors in the limiting cases of rigid inclusions and holes (see Section 3.4). Figs. 3.8 and 3.9 illustrate the distribution of stress fields around rigid inclusions of elliptical (of eccentricity 2.5:1) and irregular shapes, embedded into an infinite plane (plane stress model). Again, the plane is loaded by a remote uniaxial tension $P = 1Pa$ inclined at angle $\theta = -45^\circ$ to $x_1$ axis (see Fig. 3.10). The Young’s modulus and Poisson’s ratio of the matrix are $E_M = 10000Pa$ and $\nu_M = 0.25$, respectively.
Fig. 3.8 Elastic stress fields in the vicinity of rigid inclusions of elliptical and of irregular geometries.
Figs. 3.10 and 3.11 show these rigid inclusions, hypotrochoidal triangular and selected irregular rigid inclusions (with the properties of matrix $E_M = 10000 Pa$ and $\nu_M = 0.25$) in both the original and rotated (translated) configuration. The displaced configurations are given in a magnification of 50000:1. The inclusion boundaries are discretized using the approximating polygon with 40 to 150 vertices.

Rigid inclusions do not experience deformation and therefore only exhibit translation, rotation or a combination of these two. It is known that elliptical and triangular rigid inclusions can only exhibit rotation and translation, correspondingly (Savin, 1961). These phenomena are demonstrated in Figs. 3.10 and 3.11 on numerically calculated examples.
Fig. 3.10 Rotations/translations of rigid inclusions under uniaxial tension. The boundaries with points represent the original configurations.
(a) ellipse of eccentricity 2.5:1, (b) triangular hypotrochoid, (c) irregularly shaped inclusion.
3.3 Inclusion Compliance Contribution Tensor $H$

3.3.1 Procedure to Obtain Components of $H$ tensor

Sections 3.1 and 3.2 describe the NCM procedure to solve the elasticity problem and present solutions for some selected inclusions geometries. These results can now be directly utilized in the micromechanical procedure based on the inclusion compliance tensor $H$ described in Chapter 2.

Fig. 3.11 Rotations/translations of irregular rigid inclusions under uniaxial tension. The boundaries with points represent the original configurations.
The components of tensor $H$ can be obtained from Eq. (2.7) provided the additional strain and stress tensors, $\Delta \epsilon$ and $\Delta \sigma$, defined by Eqs. (2.6), are known. Thus, we now use the boundary tractions and displacements resulting from the solution of the elasticity problem for any direction of the uniaxial tension $\theta$, and numerically evaluate integrals in (2.6) by employing a sixteen-point Gaussian quadrature algorithm (Abramowitz and Stegun, 1965).

Repeating this procedure for various angles, we find the components of $\Delta \epsilon$ and $\Delta \sigma$ as numerical functions of $\theta$ (Fig. 2.4). The components of $H$-tensor are obtained by comparing these functions with Eqs. (2.13). We select a sufficient number of $\theta$ values and substitute them into (2.13) together with the corresponding values of $\Delta \epsilon$ and $\Delta \sigma$. This produces a system of linear equations for the components of $H$-tensor. Note that to improve accuracy of the calculation, one may choose more values of $\theta$ (we used 8 to 12) and create overdetermined system of linear equations. The components of $H$ are then found by solving this system using the least square method.

3.3.2 On Numerical Evaluation of Additional Strain and Stress

To accurately evaluate integrals in (2.6), we have to calculate the values of the differential element $d\Gamma$ of the boundary $\Gamma$ and the components of its inward unit normal $n$ (Fig. 2.3). Let us consider an inclusion of arbitrary geometry in the complex plane $z = x_i + i y_i$ with the origin inside of the inclusion, and function $\omega(\zeta)$ conformally mapping the unit disk in the canonical complex plane $\zeta$ onto the outside of the inclusion domain in the $z$ plane (Fig. 3.12).
From Muskhelishvili (1963) we have for the points on the inclusion's boundary

$$e^{i\alpha} = e^{i\theta} \frac{\omega'(\zeta)}{|\omega'(\zeta)|} = \zeta' \frac{\omega'(\zeta)}{|\omega'(\zeta)|}.$$  \hspace{1cm} (3.14)

The components of normal vector $\mathbf{n}$ follow from Eq.(3.14) immediately as

$$\mathbf{n} = \text{Re} \left[ \frac{\zeta' \omega'(\zeta)}{|\omega'(\zeta)|} \right] \mathbf{e}_1 + \text{Im} \left[ \frac{\zeta' \omega'(\zeta)}{|\omega'(\zeta)|} \right] \mathbf{e}_2.$$ \hspace{1cm} (3.15)

The expression for the differential element $d\Gamma$ can be calculated with the help of relations $d\Gamma = \sqrt{dx^2 + dy^2}$ and $z = x_1 + i y_1 = \omega'(\zeta)$ as

$$d\Gamma = \sqrt{\text{Re}[\omega'(\zeta)]^2 + \text{Im}[\omega'(\zeta)]^2} \, d\zeta = |\omega'(\zeta)| \, d\zeta.$$ \hspace{1cm} (3.16)
Our numerical computations show that with the help of expressions (3.15) and (3.16) the evaluation of line integrals in (2.6), and hence the components of tensors $\Delta \varepsilon$ and $\Delta \sigma$, is very accurate.

### 3.3.3 Elastic Inclusions

Table 3.1 presents the components of $H$-tensor calculated for elastic inclusions shown in Fig. 3.6 ($E_i = 100000\,\text{Pa}$, $E_M = 10000\,\text{Pa}$, $\nu_i = 0.05$ and $\nu_M = 0.25$). Square inclusion is shown for the illustration as well.

The procedure has also been validated by the comparison with the solution based on analytical results of Hardiman (1954) for elliptical elastic inclusion. In the case of elliptical inclusion of eccentricity 2.5:1 shown in Table 3.1 the maximum discrepancy $\delta$ evaluated as $(H_{ijkl}^{NCM} - H_{ijkl}^{Analytical})/H_{ijkl}^{Analytical}$ is less than 0.2%.

<table>
<thead>
<tr>
<th>$H_{1111}$</th>
<th>$H_{1122}$</th>
<th>$H_{1212}$</th>
<th>$H_{1122}$</th>
<th>$H_{1211}$</th>
<th>$H_{2222}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1.86E-04</td>
<td>-1.07E-04</td>
<td>-7.47E-05</td>
<td>4.11E-05</td>
<td>-1.16E-15</td>
<td>7.84E-17</td>
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<td>-1.44E-04</td>
<td>-1.44E-04</td>
<td>-9.05E-05</td>
<td>3.67E-05</td>
<td>-6.02E-13</td>
<td>-2.48E-13</td>
</tr>
<tr>
<td>-1.39E-04</td>
<td>-1.39E-04</td>
<td>-8.01E-05</td>
<td>3.87E-05</td>
<td>-4.81E-09</td>
<td>-4.86E-09</td>
</tr>
<tr>
<td>-1.45E-04</td>
<td>-1.31E-04</td>
<td>-8.58E-05</td>
<td>3.43E-05</td>
<td>-4.53E-06</td>
<td>-3.20E-06</td>
</tr>
</tbody>
</table>

Table 3.1 Components of the compliance contribution tensor $H$ for various elastic inclusions $H_{ijkl} = (A/A_i) \cdot H_{ijkl}$.  

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The numerical values of the components of $H$-tensor give full information about the contribution of inclusion to the effective elastic properties of composite. For example, $H_{1111}$ expresses the compliance of the inclusion along the $x_1$ axis. Comparison of the numerical values of $H_{1111}$ in Table 3.1 shows that, in this direction, the elliptical inclusion is considerably stiffer than the square inclusion. Full description of the properties of the resulting composites is given in Chapter 4.

### 3.3.4 Rigid Inclusions

Table 3.2 presents the components of $H$-tensor for rigid inclusions of elliptical (of eccentricity 2.5:1), hypotrochoidal triangular and of irregular shape shown in Fig. 3.10, placed in an elastic matrix having $E_M = 10000Pa$ and $\nu_M = 0.25$. Both numerical and analytical results (where available) are provided. Analytical expressions for the contribution of regularly shaped rigid inclusions can be obtained based on the results of Hardiman (1954) and Savin (1961). The effective properties of solids with such inclusions have been investigated by Jasiuk (1995) and Tsukrov (2000). Analytical expression for the components of $H$-tensor of rigid elliptical inclusion with semiaxes $a$ and $b$, oriented as shown in Table 3.2, are
\[ H_{111} = -\frac{\pi}{A E_M} \frac{2a^2 + 3ab + ab v_M^2 + 2b^2 v_M^2}{(3 - v_M)(1 + v_M)}, \]
\[ H_{222} = -\frac{\pi}{A E_M} \frac{2b^2 + 3ab + ab v_M^2}{(3 - v_M)(1 + v_M)}, \]
\[ H_{112} = -\frac{\pi}{A E_M} \frac{ab(1 - v_M^2) - 2(a + b)^2 v_M}{(3 - v_M)(1 + v_M)}, \]
\[ H_{121} = -\frac{\pi}{2AE_M} \frac{ab(a + b)^2(1 + v_M)}{a^2 + ab(1 - v_M) + b^2}. \]

(3.17)

In the case of triangular hypotrochoidal rigid inclusion,

\[ H_{111} = H_{222} = \frac{A_l}{A E_M} \frac{v_M(7 - 29v_M) - (43 + 7v_M)}{7(1 + v_M)(3 - v_M)}, \]
\[ H_{112} = \frac{A_l}{A E_M} \frac{v_M(43 + 7v_M) - (7 - 29v_M)}{7(1 + v_M)(3 - v_M)}, \]
\[ H_{121} = \frac{A_l}{A E_M} \frac{(7 - 29v_M) - (43 + 7v_M)}{14(3 - v_M)}. \]

(3.18)

<table>
<thead>
<tr>
<th>( H'_{111} )</th>
<th>( H'_{222} )</th>
<th>( H'_{112} )</th>
<th>( H'_{121} )</th>
<th>( H'_{122} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1.213E-04</td>
<td>-1.215E-04</td>
<td>-1.855E-04</td>
<td>-1.862E-04</td>
<td>-1.601E-04</td>
</tr>
<tr>
<td>4.397E-05</td>
<td>4.400E-05</td>
<td>4.724E-05</td>
<td>4.753E-05</td>
<td>4.134E-05</td>
</tr>
<tr>
<td>-9.908E-16</td>
<td>-1.008E-16</td>
<td>1.121E-12</td>
<td>1.121E-12</td>
<td>-2.865E-06</td>
</tr>
<tr>
<td>5.711E-17</td>
<td>0</td>
<td>-1.854E-12</td>
<td>0</td>
<td>-2.865E-06</td>
</tr>
</tbody>
</table>

Table 3.2 Components of the compliance contribution tensor \( \mathbf{H} \) for various rigid inclusions

\[ H_{ij}^g = \left(\frac{A}{A_l}\right) H_{ij}^g, \]
\[ \delta = \frac{H_{ij}^g - H_{ij}^\text{analytical}}{H_{ij}^\text{analytical}}. \]
Table 3.2 shows very good correspondence between the numerical and analytical results with the maximum discrepancy $\delta$ of 0.6%.

### 3.3.5 Variations of H-tensor Components with Stiffnesses Ratio

Influence of various inclusion and matrix stiffnesses can also be investigated using NCM procedure. Fig. 3.13 presents a variation of $H_{1111}$ and $H_{1212}$ for triangular elastic hypotrochoid ($v_i = 0.3$) embedded in elastic matrix having $E_M = 10^4\text{ MPa}$ and $v_M = 0.3$. The Young's modulus of the inclusion varies in the range of $E_I = 10^5$ to $10^7\text{ MPa}$.

---

**Fig. 3.13** Variation of H-tensor components for triangular hypotrochoidal inclusion with the ratio of materials’ stiffnesses.
The horizontal axis of the graph shows inclusion-to-matrix stiffness ratio $E_i/E_M$ on the logarithmic scale. The numerical results of Kachanov et al. (1994) for the hole, and Jasiuk (1995) for the rigid inclusion are indicated by stars. It can be observed that for ratios $E_i/E_M \geq 100$ and $E_i/E_M \leq 0.01$ the deviation from the analytical solution is within the range of 1%, while the results for ratios $E_i/E_M \geq 10$ and $E_i/E_M \leq 0.1$ show considerably larger deviation of 7-10%. Our conclusion is that an inclusion can be considered as rigid and as a hole, respectively, when $E_i/E_M \geq 100$ and $E_i/E_M \leq 0.01$.

3.4 Analysis of Irregularly Shaped Holes

3.4.1 Stresses Around Holes

Figs. 3.14 and 3.15 illustrate the distribution of stress fields around holes of elliptical (of eccentricity 2.5:1) and irregular shape, embedded into an infinite plane. Again, the plane is loaded by a remote uniaxial tension $P=1\, MPa$ inclined at angle $\theta=-45^\circ$ from the $x_1$ axis (see Fig. 3.16). The Young's modulus and Poisson's ratio of the matrix are $E_M=10000\, Pa$ and $\nu_M=0.25$, respectively.
Fig. 3.14  Elastic stress fields in the vicinity of elliptical hole and hole of irregular geometry in infinite plate.
Fig. 3.15 Distribution of elastic stresses along the boundary of elliptical hole and hole of irregular geometry in infinite plate.

Figs. 3.16 and 3.17 show these holes, hypotrochoidal triangular and selected irregular holes (with the properties of matrix $E_M=10000\text{Pa}$ and $\nu_M=0.25$) in both the deformed and undeformed configuration. The holes' boundaries are discretized using the approximating polygons with 40 (elliptical hole) to 180 (irregular hole, Fig. 3.17) vertices.
Fig. 3.16 Deformation of holes in infinite plane. The boundaries with points represent the undeformed configurations. (a) ellipse of eccentricity 2.5:1, (b) triangular hypotrochoid, (c) irregularly shaped hole.
3.4.2 Components of $H$ – tensor for Holes. Shape Factors

For holes, the geometry and matrix material characteristics in the expressions for the components of $H$ decouple (Kachanov et. al., 1994). Furthermore, $H$-tensor is independent of the matrix Poisson’s ratio. Thus, the material independent shape factors $h_i - h_6$ can be introduced as follows:
Examples of the numerically calculated values of $h$-factors for various regular and irregular hole shapes are presented in Table 3.3, where a comparison with finite element analysis (FEA) and analytical results is also provided.

### 3.4.3 Application of Finite Element Method to Holes

Compared to NCM, the finite element analysis (FEA) is a more universal tool: any shape can be analyzed, and an easy generalization to anisotropic materials can be made. It will be shown in this section that for the determination of $H$-tensor in the case of holes, this approach is not as precise as NCM, but with proper choice of FE mesh and discretized domain the results are reasonably accurate. The simulations have been performed using commercially available finite element program MSC.MARC.

When the finite element method is used to solve the elasticity problem for a hole under remotely applied stress field, there are several issues to be addressed: dimensions of the discretized domain, how to apply the boundary conditions, the choice of finite element mesh and how to process results of the calculations.

The FEA domain containing a defect must be large enough to minimize the interaction between its external boundaries and the boundary of a hole. On the other
hand, too large a domain leads to an excessive number of finite elements and reduces the accuracy of the calculation. To analyze the effect of the domain size on the deformation of a hole under uniaxial tension, we considered elliptical, hypotrochoidal triangular and square shapes enclosed in a square domain with the side length $D$. Let us demonstrate this analysis on an elliptical hole (of eccentricity 2.5:1). The uniaxial tension was inclined at angle $\theta = 45^\circ$ with respect to the major axis of ellipse. Two components of displacement at the tip of this axis, denoted by "$\ast"$ in Fig. 3.18, were compared against analytical solution for the tension applied at infinity (see Appendix B). Fig. 3.18 shows the dependence of results on the size of the domain. (Dotted lines correspond to the analytical solutions.)

![Fig. 3.18](image)

**Fig. 3.18** Elliptical hole under uniaxial tension at $\theta = 45^\circ$: dependence of the FEA results on the size of the discretized domain.

\[
\begin{align*}
  u_x^\ast &= \frac{u_x}{PR}, \\
  u_y^\ast &= \frac{u_y}{PR}
\end{align*}
\]
As can be seen, the square domain with the side of 8 characteristic dimensions of the defect provides sufficient accuracy in modeling the remotely applied load. Similar relation was also observed from the analysis of triangular and square holes.

Boundary conditions have to constrain the model against rigid body motion (translation and rotation) and, at the same time, not impose additional symmetries on the deformation. We tackled this problem by surrounding the domain with a layer of soft material, (having negligible stiffness as compared to the matrix material – Fig. 3.20), and applying the kinematic boundary conditions to this material. Its stiffness was chosen to be 1/1000 of the Young’s modulus of the matrix. This way of handling the boundary conditions is analogous to the penalty approach commonly used in FEA simulations.

The output from FEM analysis, namely the coordinates and displacements of the boundary nodes, is used to obtain the components of the additional strain tensor $\Delta \varepsilon$ (in the case of holes $\Delta \sigma = 0$). Based on this output, both undeformed and deformed shapes of the hole are approximated by spline functions. Then integral (2.6) is calculated using Gaussian quadrature (Abramowitz and Stegun, 1965). This is how the components of $\Delta \varepsilon$ are determined for one orientation of the loading $\theta$ (Fig. 2.4). To find $\Delta \varepsilon$ for different value of $\theta$, we re-generate the FE mesh by rotating the inner circular part of the mesh containing the hole (Fig. 3.19), and repeat the above calculations. Thus, we obtain the system of linear equations of the type (2.13). As with the NCM approach, we over-define the system by choosing more then 2 values of $\theta$ and apply the least square method to find the shape factors (3.19). The code for this procedure is written in MATLAB.
In all finite element models, we used 3-node constant strain triangular element. Our preliminary computer simulations showed that the change of element type introduces no considerable variations in the results. The number of elements in the model depends on the number of nodes on the hole boundary and fashion in which the mesh is created. All of our models were created using 80–100 boundary nodes which consequently led to the meshes having 4500–6000 elements. The examples of finite element meshes are given in Fig. 3.20.
Table 3.3 presents the NCM and FEA predictions of the shape factors for elliptical (of eccentricity 2.5:1), triangular hypotrochoidal and irregular holes. The FEA model for the elliptical hole (Fig. 3.20) consisted of 4496 linear triangular elements with 80 nodes on the hole boundary. The boundary of the irregularly shaped hole (Fig. 3.20) was discretized into 100 nodes and the total number of elements was 6539. In both cases, the side of the
domain was approximately eight times the characteristic dimension of the defect, as shown in Fig. 3.20. Analytical results (where available) are also provided for the comparison purposes. Analytical expressions for the contribution of regularly shaped holes and the effective properties of solids with holes can be obtained from Kachanov et al. (1994).
can be used to obtain the effective elastic compliances of a 3D solid with non-interacting cavities. Note that the FEM approach can also be applied to directly analyze various microstructures.

3.4.4 Compressibility of Irregularly Shaped Holes

Compressibility is the quantity that relates the pressure exerted on a body and the change in its volume. We define the compressibility of a 2-D hole, $C_{pc}$, as a relative change in its area produced by the hydrostatic loading of unit intensity. The comprehensive review of available results on compressibility of holes of various shapes can be found in Zimmerman (1991). Utilizing the hole compliance tensor $H$ and using formulas (3.19), we obtain the following expression for the compressibility of a 2-D hole:

$$C^c = \frac{1}{E_M} \left( h_1 + h_2 + 2h_4 \right)$$

(3.20)

Table 3.4 presents a comparison of the NCM predictions for hole compressibility with the analytical results of Walsh et al. (1965) and Zimmerman (1991). We have also included the results obtained using the approximate formula of Zimmerman (1991, 2001). According to this formula, the compressibility of a hole can be expressed in terms of its area $S$ and perimeter $\Pi$ as follows:

$$C_{pc} = \frac{\Pi^2 C_{pc}^0}{4\pi S}$$

(3.21)
where $C^{op}_{pe} = \frac{4(1 - \nu^2)}{E_M}$ is the compressibility of a circular hole in the case of plane strain.

<table>
<thead>
<tr>
<th>2D compressibility</th>
<th>NCM predictions</th>
<th>Analytical predictions</th>
<th>% difference NCM vs. Analytical</th>
<th>Approximate prediction</th>
<th>% difference NCM vs. Approximate</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Circular Hole" /></td>
<td>4.55E-05</td>
<td>4.55E-05</td>
<td>0.1%</td>
<td>4.33E-05</td>
<td>-5.1%</td>
</tr>
<tr>
<td><img src="image2.png" alt="Hypotrochoidal Triangular Hole" /></td>
<td>1.08E-04</td>
<td>1.08E-04</td>
<td>1.2%</td>
<td>1.18E-04</td>
<td>8.6%</td>
</tr>
<tr>
<td><img src="image3.png" alt="Irregular Hole" /></td>
<td>8.10E-05</td>
<td>-</td>
<td>-</td>
<td>8.76E-05</td>
<td>7.5%</td>
</tr>
</tbody>
</table>

Table 3.4. Compressibilities of elliptical (of eccentricity 2.5:1), hypotrochoidal triangular and irregular (Fig. 3.16) holes calculated utilizing NCM, analytical and approximate approaches.

As can be seen from the Table 3.4, NCM procedure renders data that are very close to the analytical solution (max difference is 1.2%). It is also an interesting observation that the approximate predictions yield reasonable estimates of compressibility even for highly irregular hole shapes. It supports the suggestion of Zimmerman (1991) that the hole compressibility is not very sensitive to the exact hole geometry and thus can be found with reasonable accuracy using two geometrical parameters: hole area and perimeter.
CHAPTER IV

EFFECTIVE ELASTIC MODULI OF SOLIDS WITH INCLUSIONS AND HOLES

In this Chapter, the results of the Chapters 2 and 3 are utilized to derive the effective elastic properties of matrix-based materials containing rigid inclusions, elastic inclusions and holes of irregular shapes. Mixtures of various types of heterogeneities are also considered. The results are first obtained in the approximation of non-interacting inclusions (a scheme accurate for small inclusion concentrations). The non-interacting results are then used in several first order micromechanical schemes to predict the effective properties with inclusions' interaction taken into consideration.

4.1 Solids with Many Non-Interacting Inclusions of the Same Type

This section presents the formulae for effective elastic properties of 2D solids containing elastic inclusions of identical shape. It is assumed that the location of inclusions is random and uncorrelated with their size and orientation. The predictions are obtained in the non-interaction approximation. This approximation is rigorous at small inclusion densities. As demonstrated in Chapter 2, it can also be used in some well-
developed approximate schemes to predict the effective mechanical properties of solids with interacting inclusions.

The effective moduli of solids with inclusions are expressed in terms of mechanical properties of the matrix material, components of the compliance contribution tensor and inclusion concentration (inclusion volume fraction). The inclusion concentration is defined as:

$$ f = \frac{1}{A} \sum_k A_j^{(k)} $$

(4.1)

where $A_j^{(k)}$ is the area of the $k$-th inclusion in the representative area $A$.

The non-interaction approximation of the overall compliance contribution tensor is equal to the sum of contributions $H^{(k)}$ from all inclusions (Eq. 2.15). Assuming that the local axes of all inclusions coincide with the global coordinate axes, the contribution of each $k$-th inclusion can be expressed in terms of tensor $H^*$ defined in Chapter 2 as:

$$ H^{(k)} = \frac{A_j^{(k)}}{A} H^*. $$

(4.2)

Examples of the components of $H^*$ for some inclusion shapes are given in Tables 3.1 and 3.2. The non-interaction approximation of $H$ tensor that sums the contribution of all the inclusions within RAE is expressed with the help of Eqs. (2.15), (4.1) and (4.2) as
4.1.1 Parallel Inclusions

Let us apply the procedure described in Chapter 2 to obtain the effective compliances of the material containing a set of parallel inclusions of identical shape. Utilizing Eqs. (2.14) and (4.3), the components of the effective elastic compliance tensor are:

\[
\begin{align*}
H^{ni} &= \sum H^{(k)} = \sum \frac{A_I^{(k)}}{A} H^* = f H^*. \\
4.3
\end{align*}
\]

Note that in the case of holes, one may choose to substitute expressions (3.19) and obtain the formulae in terms of the hole shape factors \( h_i \). Variation of Young’s modulus with the orientation for a solid (matrix properties: \( E_M = 20 \text{MPa} \) and \( v_M = 0.3 \) ) with parallel inclusions of irregular shape (as in Fig. 3.6c) with \( E_I = 100 \text{MPa} \) \( v_I = 0.3 \) is presented in Fig. 4.1.
The results for circular, triangular and elliptical inclusions (of eccentricity 2.5:1) are also shown for comparison. As can be observed, the curve for a material with irregular inclusions is not symmetric, suggesting that no obvious symmetry of the effective elastic tensor exists. The variation of $E/E_M$ for this material is less pronounced than that for the material with elongated (elliptical) inclusions; irregular inclusions of the shape shown in Fig. 3.6c introduce less anisotropy into the effective tensor than elliptical inclusions of eccentricity 2.5:1. Thus, deviation from isotropy is dictated by the elongation of the shape rather than the peculiarities of its geometry.

Note that isotropic behavior of composite materials is possible in the case of parallel (or non-randomly oriented) non-interacting inclusions, if the inclusions are isotropic.
objects as discussed in Chapter 2. The examples of these inclusion shapes include circles, regular polygons with the exception of squares and any arbitrarily shaped inclusions that can be mapped onto themselves by an angle different from multiples of $\pi/2$ (Tsukrov et al., 2003). The effective moduli for such materials are

\[
E = \frac{E_M}{1 + f E_M H_{1111}^*}, \quad \nu = \frac{v_M - E_M f H_{1122}^*}{1 + f E_M H_{1111}^*}.
\] (4.5)

In Fig. 4.1, there is no variation of $E/E_M$ for circular and triangular inclusion shapes. If inclusions are stiffer (softer) than matrix, circular reinforcement makes composite less (more) stiff than triangular reinforcement of the same concentration.

In the case that inclusion shapes have two perpendicular axes of geometrical symmetry, the overall properties of a material with a set of parallel inclusions are orthotropic. Its engineering constants are expressed in terms of the compliance contribution tensor as

\[
E_1 = \frac{E_M}{1 + f E_M H_{1111}^*}, \quad E_2 = \frac{E_M}{1 + f E_M H_{2222}^*},
\]
\[
\nu_{12} = \frac{v_M - E_M f H_{1122}^*}{1 + f E_M H_{1111}^*}, \quad G_{12} = \frac{E_M}{2(1 + v_M + 2f E_M H_{1212}^*)}.
\] (4.6)
4.1.2 Randomly Oriented Inclusions

Materials with \textit{randomly oriented} non-interacting inclusions exhibit isotropic behavior even in the case of highly irregular shapes (characterized by 6 independent components of \( \mathbf{H} \)). The effective Young’s modulus and Poisson’s ratio are:

\[
E = \frac{E_M}{1 + f E_M \left[ \frac{3}{8} \left( H_{1111}^* + H_{2222}^* \right) + \frac{1}{4} \left( 2H_{1212}^* + H_{1122}^* + H_{1212}^* \right) \right]}.
\]

\[
\nu = \frac{\nu_M - f E_M \left[ \frac{1}{8} \left( H_{1111}^* + H_{2222}^* \right) + \frac{3}{4} H_{1212}^* - \frac{1}{2} H_{1122}^* \right]}{1 + f E_M \left[ \frac{3}{8} \left( H_{1111}^* + H_{2222}^* \right) + \frac{1}{4} \left( 2H_{1212}^* + H_{1122}^* + H_{1212}^* \right) \right]}.
\]

For example, let us consider an elastic solid with randomly oriented inclusions of irregular shape of type shown in Fig. 3.6c with material properties of matrix and inclusions \( E_I = 100 \text{MPa}, E_M = 20 \text{MPa} \) and \( \nu_M = \nu_I = 0.3 \). The dependence of the ratio of the effective Young’s modulus of this solid to the Young’s modulus of matrix, \( E/E_M \), on the inclusion concentration is shown in Fig. 4.2. Comparison with circular and elongated elliptical shapes (\( a/b = 5 \)) shows that for randomly oriented and located non-interacting inclusions that are stiffer than the matrix, the more elongated shapes produce a higher increase in the effective stiffness.
Fig. 4.2 Effective Young's modulus as function of inclusion concentration for material with randomly oriented elastic inclusions.

4.2 Solids with Mixture of Non-Interacting Inclusions and Holes of Various Types

In this section, we consider materials with a mixture of inclusions of different shapes. The effective moduli of such materials are presented in terms of *partial inclusion concentrations*

\[
f_N = \frac{1}{A} \sum_k A_{l,N}^{(k)}
\]

(4.8)

where \(A_{l,N}^{(k)}\) refers to the area of inclusion having geometry of \(N\)-th type. If a material contains several sets of parallel inclusions with the inclusions of \(N\)-th type inclined at
angle $\alpha_N$ with respect to $x_i$ axis of the global coordinate system $x_1, x_2$, the effective compliances are as follows:

\[
S_{111} = \frac{1}{E_M} + \sum_N f_N \left[ m^4 H_{111}^* + n^4 H_{222}^* + 2m^2 n^2 (H_{1122}^* + 2H_{1212}^*) + 4m^3 nH_{1111}^* - 4mn^3 H_{1222}^* \right]_N ,
\]
\[
S_{222} = \frac{1}{E_M} + \sum_N f_N \left[ n^4 H_{1111}^* + m^4 H_{2222}^* + 2m^2 n^2 (H_{1122}^* + 2H_{1212}^*) + 4mn^3 H_{1111}^* + 4m^3 nH_{1222}^* \right]_N ,
\]
\[
S_{112} = -\frac{\nu_M}{E_M} + \sum_N f_N \left[ m^2 n^2 (H_{1111}^* + H_{2222}^*) + (m^4 + n^4)H_{1122}^* - 4m^2 n^2 H_{1212}^* + 2(m^n - mn^3)H_{1211}^* + 2(mn^3 - m^n)H_{1222}^* \right]_N ,
\]
\[
S_{121} = \frac{1 + \nu_M}{2E_M} + \sum_N f_N \left[ m^2 n^2 (H_{1111}^* + H_{2222}^*) + (m^4 - 2m^2 n^2 + n^4)H_{1112}^* + 2m^2 n^2 H_{1122}^* + 2(m^n - mn^3)H_{1211}^* + 2(mn^3 - m^n)H_{1222}^* \right]_N ,
\]
\[
S_{122} = \sum_N f_N \left[ m^2 n^2 (-H_{2222}^* + H_{1212}^* + 2H_{1122}^*) + mn^3 (H_{1111}^* - H_{1122}^* - 2H_{1212}^*) + (-n^4 - 3m^2 n^2)H_{1111}^* + (m^4 - 3m^2 n^2)H_{1222}^* \right]_N ,
\]

where $(H_{1111}^*, H_{2222}^*, ...)_N$ are the components of the compliance contribution tensor of the inclusions of $N$-th type, $m_N = \cos \alpha_N$ and $n_N = \sin \alpha_N$.

The effective elastic properties of the material with a mixture of randomly oriented inclusions are isotropic. The effective Young's modulus and Poisson's ratio are
\[ E = \frac{E_M}{1 + E_M \sum_N f_N \left( \frac{3}{8} (H_{1111}^* + H_{2222}^*) + \frac{1}{4} (2H_{1212}^* + H_{1122}^*) \right)} \]

\[ \nu = \frac{\nu_M - E_M \sum_N f_N \left( \frac{1}{8} (H_{1111}^* + H_{2222}^*) + \frac{3}{4} H_{1122}^* - \frac{1}{2} H_{1212}^* \right)}{1 + E_M \sum_N f_N \left( \frac{3}{8} (H_{1111}^* + H_{2222}^*) + \frac{1}{4} (2H_{1212}^* + H_{1122}^*) \right)} \] (4.10)

As an example, we consider the variation of Young's modulus with orientation for the material containing a mixture of randomly oriented rigid triangular inclusions and parallel elastic irregular inclusions (of type shown in Fig. 3.6c) for \( E_I = 100 \text{MPa}, \ E_M = 20 \text{MPa} \) and \( \nu_I = \nu_M = 0.3 \). The concentration of irregular inclusions is fixed at \( f_{\text{irreg}} = 0.1 \), and the concentration of triangular inclusions, \( f_{\text{tria}} \), varies from 0.05 to 0.2. Note that triangular inclusions are isotropic objects as mentioned in Chapter 2, so neither parallel nor randomly oriented inclusions of this type alone introduce any anisotropy. But, as can be seen from Fig. 4.3, the increase in the concentration of triangular inclusions in the presence of parallel inclusions raises the overall anisotropy: parameter \( \gamma = (E_{\text{max}} - E_{\text{min}})/E_M \) changes from 0.018 for \( f_{\text{tria}} = 0.05 \) to 0.024 for \( f_{\text{tria}} = 0.2 \).
4.3 Solids with Interacting Inclusions and Holes

Let us consider a two-phase composite with irregularly shaped inclusions of compliance $S_i$ homogeneously dispersed in the matrix material. It is assumed that the location of the inclusions is uncorrelated with respect to their sizes and orientations. The micromechanical predictions of the first order approximate schemes can be obtained from $H^{NI}$ as described in Chapter 2.

Fig. 4.4 shows the Mori-Tanaka and non-interaction estimates of the effective bulk modulus of the unidirectional composite (plane strain) with two phases having identical shear moduli $G_f = G_m = G = 21.739 MPa$ ($\nu_f = 0.45$ and $\nu_m = 0.15$). In this case, the components of $H$-tensor are the same for all inclusion shapes (curves for various shapes...
in Fig. 4.4 coincide), and the Mori-Tanaka prediction coincides with the analytical solution of Hill (1964) given by the following formula:

\[
K = \frac{f_f K_f (K_M + G) + (1 - f_f) K_M (K_f + G)}{f_f (K_M + G) + (1 - f_f) (K_f + G)}. \tag{4.11}
\]

Fig. 4.4 Effective bulk modulus of composite material with phases of identical shear moduli \((E_i = 63.043 \text{ MPa}, \nu_i = 0.45, E_M = 50 \text{ MPa} \text{ and } \nu_M = 0.15)\). Inclusions are stiffer than matrix.

Fig. 4.5 illustrates the application of the Mori-Tanaka and differential approximate schemes to a 2D solid with randomly oriented interacting inclusions of irregular shape shown in Fig. 3.6c \((E_i = 100 \text{ MPa} \text{ and } \nu_i = 0.3)\) inserted in a matrix material \((E_M = 20 \text{ MPa} \text{ and } \nu_M = 0.3)\). As can be seen, the Mori-Tanaka approach predicts the
most compliant response of the composite material. This result is in agreement with the observation of Dvorak and Srinivas (1999) that Mori-Tanaka estimates constitute a lower bound when inclusions are stiffer than matrix. Non-interaction prediction is also shown for the completeness.

Fig. 4.5 Predictions of the effective Young's modulus using Mori-Tanaka and differential schemes.
CHAPTER V

MICROMECHANICAL MODELING OF POROUS CARBON/CARBON COMPOSITES

The micromechanical modeling procedure presented in the previous Chapters is applied to the analysis of carbon/carbon (C/C) composite material densified by a chemical vapor infiltration (CVI) procedure. C/C composites gain a lot of attention from the researchers for their advanced mechanical and thermal properties; they are highly resistant to wear and friction, they are lightweight, retain their strength even at high temperatures and have low coefficient of thermal expansion. An interesting property of carbon-carbon composites is self-lubrication allowing the systems to “run dry”. For their remarkable properties they have great potential for many applications in the military, aerospace and automobile industries. They are very popular for use in advanced friction and heat resistant applications, such as high-performance clutches, break discs in modern fighter jets and civilian aircrafts (Ju, 1994, Benzinger et al. 1996), rocket nozzles, glass forming management material and other uses.

The Chapter begins with the general description of the unidirectional C/C composite and outlines the two-step approach to its micromechanical modeling. Microstructure of the CVI densified carbon/carbon composite and assumptions introduced to model this material are discussed in Section 5.2. In Section 5.3, the analytical formulae to evaluate contribution of fibers to the effective elastic moduli are derived. Section 5.4 employs the numerical
conformal mapping procedure and accounts for the contribution of irregularly shaped pores. The unknown effective \textit{in-situ} mechanical properties of the matrix phase are determined in Section 5.5.

5.1 Multi-Scale Approach to Micromechanical Modeling of Porous Carbon/Carbon Composites

Unidirectional C/C composites investigated in this Chapter are fabricated by chemical vapor infiltration (CVI) of carbon felts. The technology of CVI is one of the methods for obtaining carbon matrix composites with advanced mechanical and thermal properties. It consists of synthesis of carbon particles from hydrocarbon gas (a methane/hydrogen mixture) and their deposition on carbon fibers preliminarily placed in that environment. The process runs under the temperatures around 1000°C and total pressures of 20 to 30 kPa until the carbon particles deposit and form a porous carbon matrix filling the space between the fibres. Further details on the infiltration procedure and sample properties are described in Reznik et al. (2001), and Benzinger and Hüttinger (1999). It is shown that infiltration treatment results in formation of irregularly shaped pores randomly oriented in the plane perpendicular to the direction of fiber (transverse plane), as can be seen in Fig. 5.1.
The aim of the presented research is to analyze contributions of fibers and pores to the effective elastic properties with consideration of their geometry, distribution and volume fraction in the material. It is well-known in the composite material theory that elastic moduli of unidirectional composites in the longitudinal ($x_3$) direction can be predicted with good accuracy by the so-called law of mixtures (see, for example, Hashin and Rosen, 1964):

\[ E_3 = f E_{f3} + (1 - f) E_{M3}, \]  

(5.1)

where $E_3$ is the effective Young's modulus of the composite, $E_{f3}$ and $E_{M3}$ are the Young's moduli of the fiber and matrix material along the longitudinal direction, and volume concentration of fibers $f$ is defined in Eq. (4.1). A similar expression for the effective Poisson's ratios associated with the longitudinal direction, $\nu_{13}$ and $\nu_{23}$, also
exists, but its accuracy is not good. Assuming that the properties of the composite in the
direction perpendicular to the fibers (transverse direction) are isotropic, accurate derivation
of $v_{13}$ and $v_{23}$ first requires the knowledge of the effective Poisson ratio in the transverse
direction $v_t$ (Hashin and Rosen, 1964). Determination of $v_t$ is more difficult and is also
the subject of this work.

In this study, we focus on transverse effective properties utilizing the micromechanical
procedure described in Chapter 2. We choose a two-step approach as demonstrated in Fig.
5.2.

First, the contribution of fibers is accounted for by substituting the Pyro-C matrix and
carbon fibers with an equivalent matrix material (denoted by a subscript FPC – fibers and
Pyro-C). Then, irregular pores are analyzed using numerical conformal mapping technique.
In both steps, the contribution is expressed in terms of compliance contribution tensors $H$
in both the approximation of non-interacting and interacting inclusions.
5.2 Microstructure of CVI Densified Carbon/Carbon Composite

5.2.1 Structure of C/C composite on Different Length Scales

CVI densification results in the composite that consists of carbon fibers embedded in a porous matrix of pyrolytic carbon (Pyro-C). Such materials tend to have very complex microstructure and to predict their effective mechanical properties, it is necessary to analyze them on different lengths scales. The four-level hierarchical material model has been proposed in Piat and Schnack (2003). On the nanoscale, pyrolytic carbon is known to form broad variety of texture patterns that can be classified into three groups (Fig. 5.3): isotropic, low-, medium- or high-textured (Reznik and Hüttinger, 2002).

![Fig. 5.3 High-resolution TEM images of Pyro-C](image)

On the microscale, the Pyro-C matrix has a layered structure with layers arranged around fibers (Figs. 5.4 and 5.5). Each layer has different mechanical properties in the axial, radial, and circumferential directions, i.e. is anisotropic.
These layers are formed by different modifications of pyrolytic carbon as described above. The number of layers, their width, order and structure (see Fig. 5.4 and 5.5) are determined by the deposition parameters. CVI conditions also influence the geometry, size and concentration of pores that form between fibers with pyrolytic coating. In the case of random composite felts, the total porosity of 15 to 20 % and the open porosity of approximately 10.5 % have been observed by Benzinger and Hüttinger (1999).
Fig. 5.5 Fracture surfaces of CVI densified C/C composite on a 10μm length scale.
For the detailed analysis, we have chosen a specimen of the unidirectional carbon/carbon composite manufactured using the procedure described in Reznik et al. (2001), and Benzinger and Huttinger (1999). Typical micrographs, obtained using optical light microscopy (Ermel 2002), are presented in Figs. 5.6 - 5.8 on the 500 μm, 200 μm and 50 μm length scales. We observe the circular regions representing fibers surrounded by Pyro-C matrix, and large black regions of irregular shape indicating pores (cavities). The composite contains 18% ($V_{f,\text{composite}} = 0.18$) of unidirectional carbon fibers Amoco T300 having the diameter of 7 μm. The typical pore dimensions are on the order of tens of microns.
Fig. 5.6 Typical microstructure of CVI densified C/C composite on a 500μm length scale.
Fig. 5.7 Typical microstructure of CVI densified C/C composite on a 200µm length scale.
Fig. 5.8 Typical microstructure of CVI densified C/C composite on a 50μm length scale.
5.2.2 Image Analysis

The micrograph images of the composite were processed and analyzed using ColorPoint 2.0 software (www.patrilab.com). Figs. 5.9b and 5.10b,c show the examples of the original and processed images on a 500 μm and 100 μm length scales.

Fig. 5.9 Processed microstructure images on a 500μm length scale. 
(a) original microstructure images 
(b) processed images: Gray - pores, Black - FPC (fibers and Pyro-C)
Images presented in Figures 5.9, 5.10 and thirteen other 200 μm and 500 μm length scale images were analyzed to obtain the porosity \( V_p \) of the composite. The results are summarized in Table 5.1.

<table>
<thead>
<tr>
<th></th>
<th>Image 1</th>
<th>Image 2</th>
<th>Image 3,...,15</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity ( V_p )</td>
<td>32.0%</td>
<td>29.0%</td>
<td></td>
<td>29.0%</td>
</tr>
<tr>
<td>Fiber volume fraction ( V_{f,\text{composite}} )</td>
<td>18.0%</td>
<td>18.0%</td>
<td></td>
<td>18.0%</td>
</tr>
<tr>
<td>Pyro-C volume fraction ( V_{PC} )</td>
<td>50.0%</td>
<td>53.0%</td>
<td></td>
<td>53.0%</td>
</tr>
</tbody>
</table>

Table 5.1 Fiber volume fraction and porosity of C/Pyro-C composites

These estimates of porosity can be compared with the measurements of open porosity reported in Ermel et al. (2003). According to their analysis, \( V_p^{\text{open}} = 8.8\% \). Thus, our
estimates are consistent with the observation of Reznik et al. (2001) that the total porosity is considerably greater than the open porosity.

5.2.3 Modeling Assumptions

As can be seen in Figs. 5.6-5.10, pores in this composite material are randomly distributed in the transverse plane without any preferential orientation. Their shapes are highly irregular and cannot be accurately approximated by circles, ellipses or right polygons for which the analytical elasticity solutions are available. It is also observed that the location of the fibers in the transverse plane is random, so the overall elastic properties of the composite are transversely isotropic. To analyze the transverse elastic moduli of such a composite, we employ the near-field micromechanical modeling procedure based on the concept of compliance contribution tensor as described in Chapter 2. We also observe (Fig. 5.11) that pores are elongated in the direction of the fibers and therefore the plane strain model will be used to model their contribution. Also, the pyrolytic carbon matrix material, which can be high-textured and anisotropic on the nanoscale, is modeled as homogeneous and isotropic on the length scale of fibers and pores. The procedure to predict the homogenized elastic properties of the pyrolytic carbon based on its nanostructure and texture degree is presented in Piat et al. (2003).
Fig. 5.11  Microstructure of CVI densified C/C composite on 10μm and 2μm length scales.
Typical size of the pores is about 5 to 10 times greater than that of fiber cross-section. We propose that pores can be treated as being surrounded by an equivalent elastic material (FPC) consisting of Pyro-C and carbon fibers (Fig. 5.2). Section 5.4 employs the NCM technique to evaluate their contribution into the effective transverse moduli. Carbon fibers used for reinforcement of the C/C composite have a circular cross-section, and their stiffness in longitudinal and transverse directions is known. The contribution of fibers into the effective elastic moduli is investigated in the following section.

5.3 Contribution of Fibers into Effective Elastic Properties

As shown in Fig. (5.2), the first step in our modeling approach accounts for the contribution of fibers into the effective moduli by substituting the Pyro-C and carbon fibers with an equivalent homogeneous matrix (FPC) containing no pores (pores are subject to the analysis in the following section). It is therefore necessary to determine the concentration of fibers $V_f$ in FPC as

$$V_f = \frac{V_{f,\text{composite}}}{1 - V_p} = \frac{0.18}{1 - 0.29} = 0.25$$

(5.2)

5.3.1 Circular Fiber in Infinite Plane

Micromechanical modeling of the linear elastic material reinforced by unidirectional fibers of circular cross-section is based on the plane strain elasticity solution for a circular inclusion in the infinite two-dimensional solid. According to Hardiman (1954), the stress in such an inclusion subjected to remotely applied uniaxial tension $P$ (Fig. 5.12) is uniform:
\[ \sigma_f = P\left(c_1 e_1 e_1 + c_2 e_2 e_2\right) \]  
\text{(5.3)}

where \[ c_1 = \frac{\beta}{2} \frac{1 + \beta + \gamma}{\beta - \gamma (1 - 2\beta + 2\gamma)} , \quad c_2 = \frac{\beta}{2} \frac{1 - \beta + 3\gamma}{\beta - \gamma (1 - 2\beta + 2\gamma)} , \]

and \[ \beta = \frac{E_f \nu_{PC}^2}{E_{PC} (1 - \nu_f^2)} , \quad \gamma = \frac{1}{4} \left( \frac{\beta}{1 - \nu_{PC}} - \frac{1}{1 - \nu_f} \right) . \]

In Eq. (5.3), the transverse elastic properties of fibers and Pyro-C material have been assumed linearly isotropic with Young's moduli and Poisson's ratios \( E_f, \nu_f \) and \( E_{PC}, \nu_{PC} \), correspondingly.

\section*{5.3.2 Fiber Compliance Contribution Tensor}

Following Eq. (2.3), we represent the elastic compliance of the carbon fiber reinforced Pyro-C matrix as a sum of two terms:

\[ S^{(PC)} = S^{(PC)} + H^{(f)} \]  
\text{(5.4)}
where $S^{(pc)}$ is the average compliance of the pyrolytic carbon and $H^{(f)}$ is the fibers' compliance contribution tensor.

To evaluate $H^{(f)}$, we use solution (5.3) to find traction $t = \sigma_f \cdot n$ on the boundary of circular inclusion. Substituting in (2.6) and taking into account that $\Delta \varepsilon = S^{(f)} : \Delta \sigma$ (where $S^{(f)}$ is the compliance of fiber material), we can utilize Eqs. (2.7) and (2.13) to find the $H$-tensor of one circular fiber. This yields the following expressions for the components of $H^{(f)}$ in the assumption of non-interacting fibers:

$$H^{(f)} = H^f = Vf \left[ \left( \frac{1 - \nu_f^2}{E_f} - \frac{1 - \nu_{PC}^2}{E_{PC}} \right) c_1 + \left( \nu_{PC} \frac{1 + \nu_{PC}}{E_{PC}} - \nu_f \frac{1 + \nu_f}{E_f} \right) c_2 \right]$$

$$H^{(f)} = H^f = Vf \left[ \left( \frac{1 + \nu_{PC}}{E_{PC}} - \nu_f \frac{1 + \nu_f}{E_f} \right) c_1 + \left( \frac{1 - \nu_f^2}{E_f} - \frac{1 - \nu_{PC}^2}{E_{PC}} \right) c_2 \right]$$

(5.5a)

$$H^{(f)} = H^f = Vf \frac{1}{2} \left( \frac{1 + \nu_{PC}}{E_{PC}} - \frac{1 + \nu_f}{E_f} \right) (c_1 - c_2).$$

If stiffness of the fibers is much higher than that of pyrolytic carbon, they can be treated as absolutely rigid inclusions, and the corresponding formulas are provided in Tsukrov (2000).

For interacting fibers, we use the Mori-Tanaka scheme (2.16), and the following expressions for the components of fiber compliance contribution tensor are obtained:
\[ H^{(f)}_{111} = H^{(f)}_{222} = V_f \left[ \frac{d_1(c_1 + c_2)}{1-V_f (1-c_1-c_2)} + \frac{d_2(c_1-c_2)}{1-V_f (1-c_1+c_2)} \right] \]

\[ H^{(f)}_{112} = H^{(f)}_{211} = V_f \left[ \frac{d_1(c_1 + c_2)}{1-V_f (1-c_1-c_2)} - \frac{d_2(c_1-c_2)}{1-V_f (1-c_1+c_2)} \right] \]

\[ H^{(f)}_{121} = H^{(f)}_{212} = V_f \frac{d_2(c_1-c_2)}{1-V_f (1-c_1+c_2)} \]  \hspace{1cm} (5.5b)

where \( d_1 = \frac{(1-v_f - 2\nu^2_f)E_{pc} - (1-v_{pc} - 2\nu^2_{pc})E_f}{2E_{pc}E_f} \) and \( d_2 = \frac{(1+v_f)E_{pc} - (1+v_{pc})E_f}{2E_{pc}E_f} \).

### 5.3.3 Effective Properties of Fiber Reinforced Pyrolytic Carbon

The effective elastic properties of the fiber-reinforced Pyro-C matrix in a transverse plane are isotropic. If the assumption is that the fibers are non-interacting, the corresponding Young's modulus and Poisson's ratio are found from Eqs. (5.4) and (5.5a) as

\[ E_{FPC} = \frac{E_f E_{pc}}{D^2} \left\{ E_f \left[ (1+2\nu_{pc} + \nu^2_{pc}) - E_{pc} \left[ (1+2\nu_f + \nu^2_f) - E_f \left[ 2+\nu_f - \nu^2_f \right] \right] \right] V_f c_1 + + \frac{E_f \left[ 2+\nu_f - \nu^2_f \right] - E_{pc} \left[ 2+\nu_f - \nu^2_f \right] V_f c_2 \} \] \hspace{1cm} (5.6a)

\[ \nu_{FPC} = \frac{1}{D} \left\{ E_f \nu_{pc} \left[ 1+\nu_{pc} \right] - \left[ E_f \nu_{pc} \left[ 1+\nu_{pc} \right] - E_{pc} \nu_f \left[ 1+\nu_f \right] \right] V_f c_1 + + \frac{E_f \left[ 1-\nu^2_f \right] - E_{pc} \left[ 1-\nu^2_f \right] \} V_f c_2 \} \]

where \( D = \left[ E_{pc} \left[ 1+\nu_f \right] - E_f \left[ 1+\nu_{pc} \right] \right] V_f c_1 + \left[ E_f \left[ 1+\nu_{pc} \right] - E_{pc} \left[ 1+\nu_f \right] \right] V_f c_2 + E_f + \nu_{pc} E_f. \)

Similarly, in the case of Mori-Tanaka approximation for interacting fibers, the corresponding Young's modulus and Poisson's ratio are found from Eqs. (5.4) and (5.5b) as
\[ E_{FPC} = \frac{A_1 - 2A_2}{(-A_1 + A_2)^2}, \quad \nu_{FPC} = \frac{A_2}{-A_1 + A_2}, \quad (5.6b) \]

where coefficients \( A_1 \) and \( A_2 \) are expressed as

\[
A_1 = \frac{1 - \nu_{PC}^2}{E_{PC}} + \frac{V_f d_1 (c_1 + c_2)}{1 - V_f (1 - c_1 - c_2)} + \frac{V_f d_2 (c_1 - c_2)}{1 - V_f (1 - c_1 + c_2)}
\]
\[
A_2 = -\frac{\nu_{PC}^2}{E_{PC}} + \frac{V_f d_1 (c_1 + c_2)}{1 - V_f (1 - c_1 - c_2)} - \frac{V_f d_2 (c_1 - c_2)}{1 - V_f (1 - c_1 + c_2)}.
\]

To illustrate these results, let us consider carbon fibers T300 by Amoco, used in our specimen, with transverse properties \( E_f = 14.7 \text{ GPa} \) and \( \nu_f = 0.47 \) (Donnet et al., 1998) embedded into pyrolytic graphite (\( E_{PC} = 38.6 \text{ GPa}, \nu_{PC} = 0.16; \) see Papadakis and Bernstein 1963). Variation of transverse Young’s modulus of the effective matrix with fiber concentration \( V_f \) is shown in Fig. 5.13 for both non-interaction approximation and Mori-Tanaka scheme.
Fig. 5.13 Young's modulus of the effective matrix consisting of Pyro-C and carbon fibers as function of fiber concentration.

Note that in this example the transverse stiffness of carbon fibers is considerably smaller than that of pyrolytic graphite. Therefore the introduction of fibers into the composite is reducing the overall effective Young's modulus. It can also be seen that for this contrast of constituent stiffnesses \( E_f/E_{PC} = 0.38 \), the deviation in the predicted effective elastic modulus between non-interaction and Mori-Tanaka approaches is less than 7%, even at relatively high fiber volume fraction \( V_f = 0.4 \).

5.4 Contribution of Pores into Effective Elastic Properties

5.4.1 Irregular Pores in Pyrolytic Carbon

As mentioned in Chapter 5.2, the pores are considered as sufficiently long and being placed into the equivalent transversely isotropic elastic matrix (FPC). The elastic moduli of
this equivalent matrix in the transverse plane (Young's modulus $E_{FPC}$ and Poisson's ratio $\nu_{FPC}$) have been derived in Chapter 5.3. Some preliminary results of the contribution of pores into elastic moduli of C/C composites have been reported in Novak et al. (2002).

To evaluate contribution of these irregularly shaped pores into the effective elastic properties of the CVI densified C/C composites we employ the numerical conformal mapping (NCM) procedure and calculate the components of the $H$ tensor, as described in Chapter 3. Assuming that pores of each shape type are randomly distributed and randomly oriented in the plane perpendicular to the direction of fibers, the overall material is transversely isotropic. The expressions for transverse effective Young's modulus and Poisson’s ratio are obtained from Eqs. (3.17), (4.2) and (4.7) as

$$E = \frac{E_{FPC}}{1 + \sum_{N} \nu_p^{(N)} \left( \frac{3}{8} (h_1 + h_2) + \frac{1}{4} (h_3 + h_4) \right)_N}$$

$$\nu = \frac{\nu_{FPC} - \sum_{N} \nu_p^{(N)} \left( \frac{1}{8} (h_1 + h_2) + \frac{3}{4} h_4 - \frac{1}{4} h_3 \right)_N}{1 + \sum_{N} \nu_p^{(N)} \left( \frac{3}{8} (h_1 + h_2) + \frac{1}{4} (h_3 + h_4) \right)_N}$$

where $(h_1...h_4)_N$ and $\nu_p^{(N)}$ are the shape factors and porosity of the pores of $N$-th type.

Table 5.2 presents the shapes of some typical pores in Pyro-C obtained from the micrographs (some of which are presented in Figs. 5.6 – 5.10). It can be observed, that the numerical values of $h$-coefficients vary greatly for different pore shapes - they depend not only on the pore shape but also on its orientation with respect to coordinate axes.
Table 5.2  Hole shape factors of typical Pyro-C pores. \( \delta_A \) and \( \delta_B \) quantify deviation of \( A \) and \( B \) from average values.

However, for a sufficiently large number of pores of each shape randomly distributed and oriented in the material, only two combinations of these coefficients describe the contribution of each defect shape:

\[
A = \frac{3}{8} (h_1 + h_2) + \frac{1}{4} (h_3 + h_4), \quad B = \frac{1}{8} (h_1 + h_2) + \frac{3}{4} h_4 - \frac{1}{4} h_3. \tag{5.9}
\]
The analysis of calculated values of $A$ and $B$ for each shape (Table 5.2) shows surprising closeness of these parameters for different geometries of pores present in Pyro-C. We attribute this fact to the identical manufacturing process during which they were formed.

### 5.4.2 Comparison with Selected Regular Holes

Comparison of $A$ and $B$ with the corresponding parameters of selected regular shapes (Table 5.3) shows that no regular shape can be easily chosen to adequately model the contribution of Pyro-C pores to the effective properties, even in the case when pores are randomly oriented and overall properties are isotropic.

<table>
<thead>
<tr>
<th>$h_1$</th>
<th>$h_2$</th>
<th>$h_3$</th>
<th>$h_4$</th>
<th>$h_5$</th>
<th>$h_6$</th>
<th>$A$</th>
<th>$B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.916</td>
<td>6.880</td>
<td>7.962</td>
<td>-1.008</td>
<td>0.032</td>
<td>-0.027</td>
<td>6.912</td>
<td>-1.022</td>
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<tr>
<td>3.000</td>
<td>3.000</td>
<td>4.000</td>
<td>-1.000</td>
<td>0.000</td>
<td>0.000</td>
<td>3.000</td>
<td>-1.000</td>
</tr>
<tr>
<td>4.187</td>
<td>4.121</td>
<td>8.766</td>
<td>-0.241</td>
<td>0.030</td>
<td>-0.026</td>
<td>5.247</td>
<td>-1.334</td>
</tr>
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<td>1.200</td>
<td>20.99</td>
<td>12.09</td>
<td>-0.999</td>
<td>0.000</td>
<td>0.000</td>
<td>11.10</td>
<td>-0.998</td>
</tr>
</tbody>
</table>

Table 5.3. Shape factors of selected regular holes.
To demonstrate this phenomenon, Fig. 5.14 presents variation of the overall Young’s modulus with porosity for various pore shapes. It can be observed that the curves for various typical Pyro-C pores are located much closer to the “averaged pore contribution” than the curves for presented regular holes.

Fig. 5.14 Variation of Young’s modulus with porosity for various pore geometries.
5.4.3 Overall Effective Properties of Composite

Combining Eqs. (5.7), (5.8) and (5.9), the effective transverse elastic moduli of the unidirectional porous C/C composite described in Section 5.2 are

\[ E = \frac{E_{FPC}}{1 + V_p A}, \quad \nu = \frac{\nu_{FPC} - V_p B}{1 + V_p A}, \]  \hspace{1cm} (5.10)

where \( A \) and \( B \) are the average values for pore contributions (last row of Table 5.2), porosity \( V_p \) and fiber volume fraction \( V_f \) can be determined by the analysis of micrograph images (as in Table 5.1), and \( E_{FPC}, \nu_{FPC} \) are expressed in terms of mechanical properties of fibers and Pyro-C by Eqs. (5.6).

5.5 Prediction of Mechanical Properties of Pyrolytic Carbon

Microstructure of the deposited pyrolytic carbon is significantly influenced by the processing parameters (temperature, pressure, gas composition, gas flow rate etc.). Its mechanical properties are therefore related to the depositing environment (in-situ properties) and cannot be determined on a bulk material. We apply the procedure presented in the preceding sections to determine the elastic moduli of the in-situ Pyro-C matrix from the tests performed on the entire composite. A series of uniaxial tension, as well as 3- and 4-point bending tests were conducted with the composite described in Section 5.2; see Ermel et al. (2003). Examples of the typical results for stress-strain dependence in longitudinal and transverse directions are shown in Fig. 5.15.
Fig. 5.15 Results of uniaxial tension tests performed on C/C composite (adopted from Ermel et al., 2003).

The corresponding effective elastic properties of the composite are estimated as $E_l = 53.6 \text{ GPa}$, $\nu_l = 0.33$, $E_t = 4.4 \text{ GPa}$ and $\nu_t = 0.26$, where subscripts "l" and "t" refer to the longitudinal and transverse directions, correspondingly. The mechanical properties of the fibers are known from Ermel [23] and Dormet et al. [29] as $E_{lf} = 190 \text{ GPa}$, $\nu_{lf} = 0.26$, $E_{tf} = 14.7 \text{ GPa}$ and $\nu_{tf} = 0.47$. The fiber volume fraction in the equivalent matrix FPC, $V_f = 0.25$, and the porosity of the entire composite $V_p = 0.29$ were found in sections 5.3, and 5.2.2, respectively. The mechanical properties of the constituents are summarized in Table 5.4.

<table>
<thead>
<tr>
<th></th>
<th>Longitudinal direction</th>
<th>transverse direction</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ [Gpa]</td>
<td>$\nu$ [-]</td>
<td>$E$ [Gpa]</td>
</tr>
<tr>
<td>Composite</td>
<td>53.6</td>
<td>0.33</td>
</tr>
<tr>
<td>Carbon fiber</td>
<td>190.0</td>
<td>0.26</td>
</tr>
</tbody>
</table>

Table 5.4. Mechanical properties of composite material and carbon fibers.
In the longitudinal direction, the elastic stiffness of a unidirectional composite can be estimated with a reasonable accuracy by the rule of mixtures, Eq. (5.1). The Young’s modulus of the Pyro-C in this direction is then found as

\[
E_{\text{PC},l} = \frac{E_l - V_f \cdot E_f}{1 - V_p - V_f} = \frac{53.6 - 0.18 \cdot 190}{1 - 0.29 - 0.18} = 36.6 \text{ GPa.}
\]  

(5.11)

This value is in a reasonably good agreement with the experimental measurements \(E_{\text{PC},l} = 38.6 \text{ GPa}\) of Papadakis and Bernstein (1963). One must remember, however, that the properties of the pyrolytic carbon vary considerably with the change of the manufacturing parameters, so the closeness of our estimates with their ultrasonic measurements might be accidental.

In the transverse direction, the procedure is considerably more complicated. It is based on the results of Sections 5.3 - 5.5 and follows the steps presented in Fig. 5.2. First, we have to determine the Young’s modulus and Poisson’s ratio of the equivalent matrix (FPC) consisting of Pyro-C and carbon fibers. Using Eqs. (5.10) and the average pore characteristics (Table 5.2) we obtain \(E_{\text{FPC}} = 9.9 \text{ GPa}\) and \(\nu_{\text{FPC}} = 0.25\). Then, the transverse properties of Pyro-C are calculated from Eqs. (5.6a) as \(E_{\text{PC},t} = 8.5 \text{ GPa}\) and \(\nu_{\text{PC},t} = 0.16\).

As can be seen, the elastic stiffnesses of Pyro-C in the longitudinal and transverse directions differ considerably. This can be expected, as the presence of fibers during CVI densification creates preferential directions in pyrolytic carbon – an observation also supported by microscopic studies of Reznik et al. (2001).
CHAPTER VI

CONCLUSIONS

The micromechanical procedure to obtain the effective properties considered in this work utilizes the concept of the compliance contribution tensor, and was first proposed and applied to the case of solids with regular holes by Kachanov et. al (1994). We used it to model the effective properties of 2D solids with inhomogeneities (elastic inclusions, holes and rigid inclusions) of irregular shapes. First, using Eq. (2.7), the components of the compliance contribution tensor have to be found for each individual inhomogeneity. It requires the calculation of the unknown additional strain and stress tensors. The method employing numerical conformal mapping, proposed in this work, enables us to obtain these tensors for inclusions and holes of arbitrary geometries. Direct summation of compliance contribution tensors for all the inhomogeneities found in the representative area element yields the estimate of the overall compliance of the composite in the approximation of non-interacting inclusions. When inhomogeneities of one type are present in the matrix material, the effective elastic properties are expressed in terms of the inclusion concentration. Analogously, when mixtures of inhomogeneities with different geometries and material properties are present in the matrix, effective compliance is expressed in terms of the partial concentrations of inhomogeneities. As can be seen in Eqs. (2.16 - 2.19), the non-interaction results may serve as a basic
building block to obtain the estimates of the effective properties with regard to the inhomogeneities' interaction.

The proposed NCM procedure to solve the elasticity problem (and find the additional strain and stress tensors) is based on the Kolosov-Muskhelishvili complex variable approach when four complex potentials (stress functions) must be found. The solution requires the construction of the conformal mapping function in the form of Schwartz-Christoffel integral. The computationally effective and stable algorithm involves the approximation of the integrand by a truncated Laurent series. We then seek the unknown potentials in the form of the Taylor series in the matrix region, and in the series of Faber polynomials in the inclusion domain. To find the unknown coefficients in these expansions, we have to satisfy the continuity conditions for stresses and displacements across the interface between the matrix and inclusion.

Application of the procedure to the limiting cases of holes and rigid inclusions produces results that are in good agreement with known analytical solutions. The maximum observed discrepancy for the rigid inclusions is less than 1%. Comparison with the results based on Hardiman's solution for elastic elliptical inclusion yields even better accuracy of 0.2%. Also, our numerical simulations show that for the ratios $E_i/E_M \geq 100$ and $E_i/E_M \leq 0.01$, the inclusion can be considered as rigid and as a hole, respectively. In the case of holes, we also considered the application finite element method to find the components of the compliance contribution tensor. The comparison of the results shows that it is less accurate than NCM. Finite element method is, however, a universal tool and generalization to anisotropic materials and 3D is possible. Compressibility of holes was also investigated and both numerical methods were
compared with the analytical solutions of Walsh et al. (1965) and Zimmerman (1991). We observed that the compressibility of a hole is not very sensitive to the exact hole shape, and thus confirmed the result of Zimmerman that it can be approximated with a reasonable accuracy using only two parameters: hole area and perimeter.

We applied the described micromechanical approach to determine the effective properties of the in-situ pyrolytic carbon phase of carbon/carbon composite material. A two-step methodology was proposed. In the first step, we substituted fibers and in-situ pyrolytic carbon with an equivalent homogeneous matrix. The contributions of fibers to the effective properties were evaluated in closed form, and this yielded the explicit expressions for elastic moduli of the fiber reinforced composite material. In the second step, we applied the numerical conformal mapping technique to analyze the contribution of irregular pores. We observed that the numerical parameters describing the contributions of various pyrolytic carbon pores to the effective properties were relatively close. We attribute this phenomenon to the identical manufacturing procedure during which they were formed. The corresponding parameters for selected regular pore shapes were noticeably different. Our conclusion is that there is no obvious way to approximate irregular pores in the composite by regular shapes without considerable loss of accuracy. The obtained properties of in-situ pyrolytic carbon show that CVI densification of the unidirectional C/C composite results in the formation of pyrolytic carbon that has different mechanical properties in the longitudinal and transverse direction. Therefore, not only the resulting composite, but also the matrix cannot be modeled as isotropic material.


Chen-Chi M. Ma, Nyan-Hwa Tai, Wen-Chi Chang, Yi-Pin Tsai, 1996. Morphologies, microstructures and mechanical properties of 2D carbon/carbon composites during the CVI densification process. Carbon 34, 1175-1179.


Lee, J.K., Johnson, W.C., 1977. Elastic strain energy and interactions on thin square plates which have undergone a simple shear. Scripta Metallurgica 11, 477-484.


SIMPLIFICATIONS TO H-TENSOR

As discussed in Chapter 2, H-tensor can be simplified for certain inclusion geometries. Below we consider several special cases when the number of the independent components can be reduced.

- **Case 1. Inclusions with two perpendicular axes of symmetry**
  In this case, the components of both $\sigma$ and $\Delta\varepsilon$ tensors should not change when the coordinate axes are rotated by 180 degrees. Using the Eq. (2.7) for $\Delta\varepsilon_{ij}$ ($\Delta\sigma_{ij}$ part of this equation is omitted for the symmetry consideration since it has identical structure to $\Delta\varepsilon_{ij}$) in both the original and the rotated orientations of the axes, we obtain the following equations:

  for $i = j$
  \[
  H_{\hat{y}11}\sigma_{11} + H_{\hat{y}12}\sigma_{12} + H_{\hat{y}21}\sigma_{12} + H_{\hat{y}22}\sigma_{22} = H_{\hat{y}11}\sigma_{11} - H_{\hat{y}12}\sigma_{12} - H_{\hat{y}21}\sigma_{12} + H_{\hat{y}22}\sigma_{22}
  \]
  and for $i \neq j$
  \[
  H_{\hat{y}11}\sigma_{11} + H_{\hat{y}12}\sigma_{12} + H_{\hat{y}21}\sigma_{12} + H_{\hat{y}22}\sigma_{22} = -H_{\hat{y}11}\sigma_{11} + H_{\hat{y}12}\sigma_{12} + H_{\hat{y}21}\sigma_{12} - H_{\hat{y}22}\sigma_{22}
  \]  
  (A.1)

  Taking into account the symmetry condition $H_{\hat{y}lm} = H_{\hat{m}lk} = H_{\hat{k}lj}$ we observe that Eqs. (A.1) can only be satisfied when $H_{\hat{y}11} = H_{\hat{y}22} = 0$ for $i \neq j$ and $H_{\hat{y}12} = H_{\hat{y}21} = 0$ for $i = j$.

  This implies that $H_{1222} = H_{1211} = 0$, reducing the number of independent coefficients to four.

- **Case 2. Inclusion symmetrical with respect to 90 degree rotation (for example, square inclusions)**
  In this case (inclusion that superimposes upon itself after each 90 degree rotation), the components of $\sigma$ and $\Delta\varepsilon$ tensors must remain unchanged for every 90 degree rotation.
This yields

\[ H_{1111}\sigma_{22} + H_{1122}\sigma_{11} = H_{2211}\sigma_{11} + H_{2222}\sigma_{22} \]  \hspace{1cm} (A.2)

To satisfy the above equation one must set $H_{1111} = H_{2222}$, further reducing the number of the independent coefficients to three.

- **Case 3. Inclusion symmetrical with respect to 45 degree rotation**

Similarly, as in the previous cases we require that both $\sigma$ and $\Delta\epsilon$ tensors have equal components after each such rotation of the inclusion shape. This implies that

\[
\sigma_{11}\left(\frac{1}{2}H_{1111} + \frac{1}{2}H_{2211}\right) + \sigma_{12}\left(H_{1212} + H_{1221}\right) + \sigma_{22}\left(\frac{1}{2}H_{1122} + \frac{1}{2}H_{2222}\right) = \\
= \sigma_{11}\left(\frac{1}{2}H_{1111} + \frac{1}{2}H_{1122}\right) + \sigma_{12}\left(H_{1111} - H_{1122}\right) + \sigma_{22}\left(\frac{1}{2}H_{1111} + \frac{1}{2}H_{1122}\right) 
\]  \hspace{1cm} (A.3)

From the case 1 and 2 above it is known that the terms following $\sigma_{11}$ and $\sigma_{22}$ are equal. Thus to satisfy Eq. (A3) we must set $H_{1212} = (H_{1111} - H_{1122})/2$, which implies, that

\[ H_{1212} = \frac{H_{1111} - H_{1122}}{2} = \frac{H_{2222} - H_{1122}}{2}. \]

This reduces the number of the independent coefficients to two.

Tsukrov et al. (2003) further showed that relationship (A.3) holds also in the case of the shapes that are symmetrical with respect to the rotation other than 90 and 180 degrees (for example equilateral triangles).
Solution of this problem was given by many authors using various methods. The one used for our comparison analysis is published in Muskhelisvili (1963), and is presented here for the sake of completeness. The conformal mapping \( z = R(\zeta + m/\zeta) \) is used to map the infinite plane with an elliptical hole having semiaxes \( a \) and \( b \) onto the exterior of a unit circle in the canonical complex plane \( \zeta \). The displacements and stresses are then expressed in terms of two analytic complex functions

\[
\varphi(\zeta) = \frac{PR}{4} \left( \zeta + \frac{2e^{2i\theta} - m}{\zeta} \right),
\]

\[
\psi(\zeta) = -\frac{PR}{2} \left( e^{-2i\theta} \zeta + \frac{e^{2i\theta}}{m\zeta} - \frac{(1 + m^2)(e^{2i\theta} - m)}{m} \frac{\zeta}{\zeta^2 - m} \right),
\]

where \( R = (a + b)/2 \), \( m = (a - b)/(a + b) \) and \( P \) is the stress applied at infinity and inclined at angle \( \theta \) to the major semiaxis. The displacements on the boundary of the hole can then be determined from Eq. (3.3).

Substituting Eq. (B.1) into Eq. (3.3) and separating real and imaginary parts we obtain, after some algebraic operations, the following expressions for the displacements

\[
u = \frac{PR}{E_M}\left(1 - \nu_M^2\right)\left[(1 - m)\cos \gamma + 2(\cos 2\theta \cos \gamma + \sin 2\theta \sin \gamma)\right]
\]

\[
v = \frac{PR}{E_M}\left(1 - \nu_M^2\right)\left[(1 + m)\sin \gamma - 2(\cos 2\theta \sin \gamma - \sin 2\theta \cos \gamma)\right],
\]
where $u$ and $v$ are the components of displacement at the point on the boundary of an elliptical hole that corresponds to point $\zeta = e^{i\eta}$ in the canonical plane $\zeta$.

The components of displacement at the tip of the major axis of ellipse ($b/a = 1/2.5$) when remote loading is inclined at $\theta = 45^\circ$ and $\nu_m = 0.3$ are

$$u = 0.52 \frac{PR}{E_m}$$

$$v = 1.82 \frac{PR}{E_m}.$$
EVALUATION OF LIMITS IN EQ. (3.8)

Substituting Eqs. (3.1), (3.2) and (3.7) into the first limit in Eqs. (3.8) we obtain

\[
\lim_{\zeta \to 0} \left( u_o^M + i v_o^M \right) =
\]

\[
= \lim_{\zeta \to 0} \left\{ \frac{3 - v_M}{E_M} \varphi_{M,o}(\zeta) - \frac{1 + v_M}{E_M} \left[ \frac{\omega(\zeta)}{\omega' \varphi_{M,o}(\zeta)} + \psi_{M,o}(\zeta) \right] \right\} =
\]

\[
\lim_{\zeta \to 0} \left\{ \frac{3 - v_M}{E_M} \sum_{n=0}^{\infty} c_n^M \zeta^n - \frac{1 + v_M}{E_M} \left[ \sum_{n=0}^{\infty} n a_n^M \zeta^{n-1} + \sum_{n=0}^{\infty} \beta_n^M \zeta^n \right] \right\} =
\]

\[
\lim_{\zeta \to 0} \left\{ \frac{3 - v_M}{E_M} \sum_{n=0}^{\infty} c_n^M \zeta^n - \frac{1 + v_M}{E_M} \left[ \sum_{n=0}^{\infty} n a_n^M \zeta^{n-1} + \sum_{n=0}^{\infty} \beta_n^M \zeta^n \right] \right\} =
\]

\[
\frac{3 - v_M}{E_M} \alpha_0^M - \frac{1 + v_M}{E_M} \beta_0^M = \frac{1 + v_M}{E_M} \left( \frac{3 - v_M}{E_M} \alpha_0^M - \beta_0^M \right).
\]

Substituting Eqs. (3.1), (3.2) and (3.7) into the second limit in Eqs. (3.8) we obtain

\[
\lim_{\zeta \to 0} \left( \sigma_{xx,o}^M + \sigma_{yy,o}^M \right) = \lim_{\zeta \to 0} \left\{ 4 \text{Re} \frac{\varphi_{M,o}'(\zeta)}{\omega'(\zeta)} \right\} =
\]

\[
= \lim_{\zeta \to 0} \left\{ 4 \text{Re} \frac{1}{\sum_{j=-2}^{M} a_j \zeta^j} \right\} = \lim_{\zeta \to 0} \left\{ 4 \text{Re} \frac{\sum_{n=0}^{\infty} n a_n^M \zeta^{n-1}}{\zeta^2 + O(1)} \right\} = 0. \quad \text{(C.2)}
\]
Finally, substituting Eqs. (3.1), (3.2) and (3.7) into the last limit in Eqs. (3.8) we obtain

\[
\lim_{\zeta \to 0} \left( \sigma_{yy,0}^M - \sigma_{xv,0}^M + 2i \tau_{xy,0}^M \right) =
\]

\[
= \lim_{\zeta \to 0} 2 \left( \frac{\varphi_{M,0}(\zeta)}{\omega'_{M,0}(\zeta)} - \varphi'_{M,0}(\zeta) \frac{\omega''(\zeta)}{\omega^2(\zeta)} + \frac{\psi'_{M,0}(\zeta)}{\omega'(\zeta)} \right)
\]

\[
= \lim_{\zeta \to 0} \left[ \sum_{n=0}^{\infty} \frac{n(n-1)\alpha_n^M \zeta^{-n-2}}{\sum_{j=0}^{M} a_j \zeta^j} - \sum_{n=0}^{\infty} \frac{n\alpha_n^M \zeta^{-n-1}}{\sum_{j=0}^{M} a_j \zeta^j} \sum_{j=0}^{M} j a_j \zeta^j \right]
\]

\[
+ \sum_{n=0}^{\infty} \frac{n \beta_n^M \zeta^{-n-1}}{\sum_{j=0}^{M} a_j \zeta^j} =
\]

\[
= \lim_{\zeta \to 0} \left[ \sum_{n=0}^{\infty} \frac{n(n-1)\alpha_n^M \zeta^{-n-2}}{\frac{1}{\zeta^4} + O(\zeta^{-3})} - \sum_{n=0}^{\infty} \frac{n\alpha_n^M \zeta^{-n-1}}{\frac{1}{\zeta^3} + O(\zeta^{-2})} \left( \frac{1}{\zeta^3} + O(\zeta) \right) + \sum_{n=0}^{\infty} \frac{n \beta_n^M \zeta^{-n-1}}{\frac{1}{\zeta^2} + O(1)} \right]
\]

\[
\]

\[
= 0
\]