An investigation on flow field partitioning related to the rheological heterogeneities and its application to geological examples

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Abstract

Earth’s lithosphere is heterogeneous and composed of rheologically distinct elements at various scales of observations. This causes the flow of rocks to vary with space and time, which may influence the formation of various kinds of geological rock records. This thesis provides quantitative solutions to some first-order problems in structural geology regarding this heterogeneous flow variation and thereby the development of various geological rock records at different scales of observations.

Pressure in a rheologically heterogeneous element may deviate from its ambient value and if significant, may influence the metamorphic assemblages. This might cause problems in the routine use of geothermobarometry-based pressure estimates from mineral assemblages as a proxy for depth in geodynamic models of geological processes. A micromechanics-based multiscale model called Multi Order Power Law Approach (MOPLA) is applied to simulate pressure deviation in and around a rheologically distinct rock element embedded in a rock medium of a non-linear viscous anisotropic rheology. The results show that the pressure deviations are in the same order as the deviatoric stress levels and hence limited by the strength of rocks.

Flow variation can influence c-axis fabrics from quartz aggregate within feldspar-mica matrix in the natural high strain zones. If such effect is not accounted for, crucial geological information such as deformation temperature, deformation history and shear sense obtained using c-axis fabrics can be seriously misinterpreted. A multiscale approach coupling MOPLA with Viscoplastic Self-consistent (VPSC) model is used to simulate c-axis fabrics under partitioned flow. The results show that the quartz c-axis fabric variation showing apparent opposite senses of shear within a single thin section, can be explained by partitioned flow within the quartz domains and reflect finite strain gradient rather than a reversal of vorticity sense as previously thought.

Flow variation can form flanking structures around a cross-cutting element like a vein or a dyke that may provide kinematic information such as ‘shear sense’ and ‘finite strain’. Their correct interpretations are critical for understanding regional tectonics. A micromechanics-
based modeling approach is used to simulate 3-D flanking structures and demonstrate how the flanking structure may vary with the cutting element’s shape, orientation, and rheological contrast to the ambient medium. A reverse-dynamic modeling approach is applied to quantitatively estimate kinematic vorticity number, viscosity contrast of the cutting element to the ambient medium, and finite strain from natural flanking structures.

Keywords
Micromechanics, MOPLA, pressure deviation, VPSC, c-axis fabrics, flanking structures, ductile shear zones, numerical modeling.
Summary for Lay Audience

Earth’s lithosphere is continually subjected to forces that deform rocks and form patterns or structures of characteristic lengths ranging from crystal-scale to the scale of a lithospheric plate. Studying these geological structures can provide information about underlying geodynamic processes. However, field observations of geological structures can only allow access to few scales ranging from rock outcrops to hand specimens, to microscopic thin sections. A scale gap exists between the field observations and the tectonic processes that occur at the orogenic or plate boundary scale. Since the lithosphere is heterogeneous and composed of rheologically distinct elements, the flow in the rocks can vary, a phenomenon called flow partitioning. The geological structures from field observations are, therefore, relevant to the partitioned flow at the respective scales and cannot be directly linked to the tectonic scale processes. This thesis applies micromechanics-based numerical models to simulate such multiscale rock deformation in Earth’s lithosphere.

This thesis provides a quantitative understanding of geological phenomena due to the heterogeneous deformation of Earth’s lithosphere. Pressure may deviate in and around any rheologically heterogeneous rock element and may influence metamorphic assemblages. This can cause problems in using pressure-depth relationships in geodynamic models. Pressure deviations in and around the heterogeneous rock element were simulated and it was found that the pressure deviations are in the same order as the deviatoric stress levels in rocks and hence limited by their strength. Flow variation in quartz aggregates can influence c-axis fabrics and cause problems in their interpretation. Quartz c-axis fabrics were simulated under partitioned flow and it was found that the c-axis fabric variation showing apparent opposite senses of shear within a single thin section reflects a finite strain gradient rather than a reversal of vorticity sense as previously thought. Flow variation around any cross-cutting rock element such as a dyke, can form flanking structures, which are useful tools to infer kinematic information such as finite strain and shear sense. 3-D flanking structures were simulated, and it was demonstrated how flanking structures may vary with cutting element’s viscosity, 3-D shape, and orientation, as well as finite strains. A computer program is developed to quantitatively estimate kinematic information such as cutting element’s viscosity, finite strain, and kinematic vorticity number from a photograph of a natural flanking structure.
Co-Authorship Statement

An earlier version of Chapter 3 in this thesis was published as a co-authored paper “Pressure variations among rheologically heterogeneous elements in Earth's lithosphere: A micromechanics investigation”. In Earth and Planetary Science Letters, 498, 397-407. (https://doi.org/10.1016/j.epsl.2018.07.010). The authors of this paper are Jiang, D, and Bhandari, A. D. Jiang conceived and designed the analysis, provided the programming code and assistance with interpretation of the data, wrote the manuscript. A. Bhandari carried out the literature review, developed the additional MATLAB code for anisotropic medium case, performed the numerical simulations, visualized the data, wrote initial versions of the manuscript, and edited the final manuscript.

Chapter-4 in this thesis was published as a co-authored paper “A multiscale numerical modeling investigation on the significance of flow partitioning for the development of quartz c-axis fabrics” in Journal of Geophysical Research: Solid Earth, 126, e2020JB021040. (https://doi.org/10.1029/2020JB021040). The authors of this paper are Bhandari, A, and Jiang, D. D. Jiang conceived and designed the analysis, provided the programming code and assistance with interpretation of the data, thoroughly edited the manuscript. A. Bhandari developed the additional parts of MATLAB code, performed the numerical simulations, visualized the data, wrote the manuscript.

Chapter- 5 is a co-authored manuscript. The authors of these manuscripts are Bhandari, A, and Jiang, D. D. Jiang conceived the analysis, provided the initial version of programming code and assistance with interpretation of the data, thoroughly edited the manuscript. A. Bhandari designed the analysis, developed the additional parts of MATLAB code, performed the numerical simulations, visualized the data, wrote the manuscript.
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Nomenclature

Symbol quantities

\( a_1, a_2, a_3, a_i \)  
the semi-axis of an ellipsoid (first, second, third, general)

\( A, A_{ijkl} \)  
Strain rate partitioning tensor, components (fourth-order)

\( \varepsilon, \varepsilon_{ij} \)  
Elastic strain or viscous strain rate tensor in the ellipsoidal inclusion, components (second-order)

\( \varepsilon(x), \varepsilon_{ij}(x) \)  
Elastic strain or viscous strain rate tensor around the ellipsoidal inclusion or RDE as a function of position vector \( x \), components (second-order)

\( E, E_{ij} \)  
Elastic strain or viscous strain rate tensor in the far-field matrix or HEM, components (second-order)

\( w, w_{ij} \)  
Elastic rotation tensor or vorticity in the ellipsoidal inclusion or RDE stated in the reference frame tracking ellipsoid axes, components (second-order)

\( w(x), w_{ij}(x) \)  
Elastic rotation tensor or vorticity around the ellipsoidal inclusion or RDE as a function of position vector \( x \) stated in the reference frame tracking ellipsoid axes, components (second-order)

\( W, W_{ij} \)  
Elastic rotation tensor or vorticity of the far-field matrix or HEM, components (second-order)

\( \sigma, \sigma_{ij} \)  
Cauchy stress tensor or deviatoric stress tensor in the ellipsoidal inclusion or RDE, components (second-order)

\( \sigma(x), \sigma_{ij}(x) \)  
Cauchy stress tensor or deviatoric stress tensor around the ellipsoidal inclusion or RDE as a function of position vector \( x \), components (second-order)

\( \Sigma, \Sigma_{ij} \)  
Cauchy stress tensor or deviatoric stress tensor in the far-field matrix or HEM, components (second-order)

\( C, C_{ijkl} \)  
Elastic moduli or viscous stiffness tensor, components (fourth-order)

\( p \)  
The pressure inside the inclusion or RDE

\( p(x) \)  
Pressure around the inclusion or RDE as a function of position vector \( x \)

\( P \)  
Pressure in the far-field matrix or HEM

\( P_L \)  
Lithostatic pressure

\( \tilde{p}_0 \)  
Initial pressure deviation in the spherical inhomogeneity

\( \tilde{p}_r \)  
Equilibrated residue pressure deviation in the spherical inhomogeneity

\( \mu \)  
Elastic shear modulus of the embedding matrix

\( K^* \)  
The bulk modulus of the inhomogeneity
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<tbody>
<tr>
<td>$\mathcal{D}$</td>
<td>The characteristic length of the crustal deformation zone</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Fluctuation length of the boundary loading and velocity conditions</td>
</tr>
<tr>
<td>D</td>
<td>Macroscale characteristic length</td>
</tr>
<tr>
<td>d</td>
<td>Mesoscale characteristic length</td>
</tr>
<tr>
<td>$\delta$</td>
<td>Microscale characteristic length</td>
</tr>
<tr>
<td>$S, S_{ijkl}$</td>
<td>Symmetric Eshelby tensor for incompressible viscous materials, components (fourth-order)</td>
</tr>
<tr>
<td>$\Pi, \Pi_{ijkl}$</td>
<td>Anti-symmetric Eshelby tensor for incompressible viscous materials, components (fourth-order)</td>
</tr>
<tr>
<td>$\Lambda, \Lambda_{ij}$</td>
<td>Auxiliary tensor for pressure field (second-order)</td>
</tr>
<tr>
<td>$J^d$</td>
<td>Fourth Order deviatoric identity tensor</td>
</tr>
<tr>
<td>$J^s$</td>
<td>Fourth Order anti-symmetric identity tensor</td>
</tr>
<tr>
<td>$\delta_{ij}$</td>
<td>Kronecker delta</td>
</tr>
<tr>
<td>$T, T_{ijkl}$</td>
<td>Green interaction tensor for incompressible viscous materials (fourth-tensor)</td>
</tr>
<tr>
<td>$G_y(x)$</td>
<td>Green function for velocity</td>
</tr>
<tr>
<td>$H_z(x)$</td>
<td>Green function for pressure</td>
</tr>
<tr>
<td>$G_{y;i}(x)$</td>
<td>Spatial derivative of the Green function for velocity</td>
</tr>
<tr>
<td>L</td>
<td>Velocity gradient tensor of matrix flow (second-order)</td>
</tr>
<tr>
<td>n</td>
<td>Power Law stress exponents</td>
</tr>
<tr>
<td>$\eta$</td>
<td>normal viscosity for the resistance to pure shearing along and perpendicular to the layering</td>
</tr>
<tr>
<td>$\eta_s$</td>
<td>shear viscosity measuring the resistance to shearing parallel to the layering</td>
</tr>
<tr>
<td>m</td>
<td>Strength of planar anisotropy</td>
</tr>
<tr>
<td>r</td>
<td>The ratio of inclusion’s viscosity to that of the ambient medium, or HEM.</td>
</tr>
<tr>
<td>$W_i$</td>
<td>Kinematic vorticity number</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Finite strain intensity</td>
</tr>
</tbody>
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**Super- or sub-script labeling**

<table>
<thead>
<tr>
<th>Superscript</th>
<th>Description</th>
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<tbody>
<tr>
<td>eff</td>
<td>Effective</td>
</tr>
<tr>
<td>in</td>
<td>Ellipsoidal inclusion or RDE</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>------------------------</td>
</tr>
<tr>
<td>$E$</td>
<td>Exterior Eshelby field</td>
</tr>
<tr>
<td>M</td>
<td>Matrix</td>
</tr>
<tr>
<td>iso</td>
<td>isotropic material</td>
</tr>
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### Acronyms

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tr>
<td>HEM</td>
<td>Homogenous Effective Medium</td>
</tr>
<tr>
<td>MOPLA</td>
<td>Multi Order Power Law Approach</td>
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<tr>
<td>RDE</td>
<td>Rheologically Distinct Element</td>
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<td>RVE</td>
<td>Representative Volume Element</td>
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<td>VPSC</td>
<td>Viscoplastic self-consistent</td>
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Chapter 1

1 General Introduction and Thesis Outline

1.1 Introduction

Earth’s lithosphere is continually subjected to forces that cause deformation in rocks and result in the formation of patterns or structures of characteristic lengths ranging from crystal-scale to the scale of a lithospheric plate. Structural geology and tectonics deal with the systematic study of these geological structures to understand the underlying geodynamic processes (e.g., Twiss and Moores, 1992; Passchier and Trouw, 2005). However, field observations of geological structures allow easy access to only a few scales ranging from rock outcrops to hand specimens, to microscopic thin sections. A scale gap exists between the field observations and the tectonic processes that occur at the orogenic or plate boundary scale. A classical continuum mechanics approach has been extensively used to interpret the relationship between the geological structures and the associated flow fields to unravel the geological history of the deforming zones (e.g., Hobbs et al., 1976; Twiss and Moores, 1992; Pollard and Fletcher, 2005). Some examples of continuum mechanics models include single or multi-layer folding models of Johnson and Fletcher (1994), Schmalholz and Podladchikov (2000), Hudleston and Treagus (2010), and Schmalholz and Schmid (2012); models for the formation of pinch-and-swell structures Smith (1977), Schmalholz et al. (2008), Schmalholz and Fletcher (2011), shear zone model of Ramsay and Graham (1970) and Ramberg (1975); transpressional zone model of Robin and Cruden (1994); Taylor-Bishop-Hill model of Lister and Hobbs (1980) and viscoplastic self-consistent (VPSC) model of Lebensohn and Tome (1993) for development of c-axis fabrics. These investigations analyze specific structures of a single or limited characteristic length scale and hence are referred to as single-scale models (Jiang 2014). Since the classical continuum mechanics do not have parameters with length scales, one cannot investigate different characteristic scales in a single problem with this approach.

Earth’s lithosphere is heterogeneous and composed of rheologically distinct elements (RDEs). These RDEs can occur over a wide range of scales of observation e.g., a pluton
at the tectonic scale (Bentley, 2004), eclogite lenses at the outcrop scale (O’Brien 2018), or quartz aggregates (Kilian et al., 2011) at thin-section scale (Fig. 1.1). Deformation of such heterogeneous rock mass may cause mechanical fields such as deviatoric stress, strain rate, vorticity, and pressure to vary from one RDE to another and thereby influence the formation of geological rock records (e.g., Lister and Williams, 1983; Jiang, 1994; Jiang and White, 1995; Jiang and Williams, 1999; Goodwin and Tikoff, 2002; Jones et al., 2005; Jiang and Bentley, 2012; Jiang, 2014; Yang et al., 2019). Such flow variation due to RDEs is known as ‘flow partitioning’ (Lister and Williams, 1983). The geological structures from field observations are relevant to the partitioned flow at the respective scales and cannot be directly linked to the tectonic scale processes. While many geologists have realized this problem, none of the existing single-scale models can address the multiscale deformation of the heterogeneous lithosphere.

Flow partitioning lies at the heart of some of the most fundamental problems in structural geology. For example, the pressure within or around an RDE may deviate from its ambient value (Gerya, 2015) and if significant, may influence the metamorphic assemblages in the RDE. This might cause problems in the routine use of geothermobarometry-based pressure estimates from mineral assemblages as a proxy for depth in geodynamic models of geological processes. Flow partitioning can also cause problems in the interpretation of c-axis fabric data from an RDE such as quartz aggregates within feldspar-mica matrix in the natural high strain zones. Strain rate and vorticity variation within the RDE affect quartz c-axis fabric formation throughout geological history. If such an effect is not accounted for, crucial geological information such as deformation temperature, deformation history, and shear sense, which is widely obtained by structural geologists using the c-axis fabric data, can be seriously misinterpreted. Flow partitioning is also responsible for the formation of ‘flanking structures’ (Passchier, 2001), which are deflections in planar or linear fabric elements around a cross-cutting element like a vein or a dyke in ductile shear zones. Strain rate and vorticity variation around and in the close vicinity of a cutting element can form different kinds of flanking structures, which provide useful kinematic information.
Figure 1.1. Rheological heterogeneities in Earth’s lithosphere at various scales of observation (a) Regional map of the Sierra Crest shear zone system and surrounding rocks, showing different rheologically distinct rock units (with different color) at tectonic scale (modified after Bentley, 2004) (b) Thin-section microphotograph showing quartz aggregates embedded in feldspar-mica matrix from Gran Paradiso Metagranodiorite shear zones, Italy (modified after Kilian et al., 2011) (c) Outcrop scale picture of eclogite boudins in Puga Gneiss, NW Himalayas. The geologist circled in the left foreground is for scale (modified after O’Brien, 2018).
such as ‘shear sense’ and ‘finite strain’. Their incorrect interpretation can lead to serious
errors in understanding regional tectonic processes (Grasemann et al., 2018). These
examples clearly show how flow partitioning might affect the formation of geological
rock records at different scales of observation. To better understand the multiscale
dynamics of the lithosphere, it is highly critical to study how and to what extent
rheological heterogeneities influence the mechanical behavior, and hence the imprinting
structural rock record in Earth’s lithosphere. The main objective of this thesis is to
understand this heterogeneous deformation of Earth’s lithosphere and provide solutions
to first-order problems in structural geology such as pressure variation among
rheologically heterogeneous elements in Earth’s lithosphere, the influence of flow
partitioning on quartz c-axis fabrics from natural shear zones and the development of
flanking structures around a cross-cutting element in ductile shear zones. A multiscale
approach is required for this purpose.

In recent years, a new micromechanics-based approach called Multi Order Power Law
Approach (MOPLA, Jiang and Bentley, 2012; Jiang, 2012, 2016; Qu et al., 2016; Lu,
2020) has been developed to address the multiscale deformation of Earth’s lithosphere.
The theoretical basis of MOPLA lies in the seminal work of Eshelby (1957,1959), who
solved for the elastic field inside and around an ellipsoidal inclusion embedded in an
infinite homogenous elastic medium (Fig.1.2). In subsequent years, the solutions to the
Eshelby inclusion problem have been extended to general elastic inclusions (Mura, 1987)
and then, to general non-linear power-law viscous materials (Molinari, 1987; Lebensohn
and Tome, 1993; Jiang and Bentley, 2012; Jiang, 2013, 2014). In MOPLA, each RDE in
Earth’s lithosphere is regarded as an ellipsoidal inclusion embedded in a macroscale
viscous medium, subjected to a far-field deformation (Fig. 1.3a-d). Although the
macroscale viscous medium is rheologically heterogeneous, in MOPLA, it is represented
by a homogeneous-equivalent medium (HEM) (e.g. Jiang, 2014; Lebensohn and Tomé,
1993) whose rheology is obtained self-consistently using homogenization from the
rheological properties of all constituent elements contained in the representative volume
element (RVE) with which the macroscale flow is defined (Fig.1.3d). The local
mechanical fields, such as deviatoric stress, strain rate, vorticity, and pressure, are
partitioned from the respective far-field quantities and are responsible for fabric
development at the local scale (Fig. 1.3e, f, g). The numerical simulations are realized
using MATLAB scripts, whose algorithms are available in the literature (e.g., Jiang,
2014; Jiang, 2016; Qu et al., 2016; Lu, 2020). The goal of this thesis is to apply and
further develop MOPLA for application to specific problems in structural geology.

Figure 1.2 An illustration of Eshelby inclusion problem of an ellipsoidal elastic
inclusion embedded in an infinite homogeneous elastic medium. \( \varepsilon \), \( w \), and \( \sigma \) are
the uniform elastic strain, rotation, and Cauchy stress fields inside the inclusion.
\( \varepsilon(x), w(x), \) and \( \sigma(x) \) are the elastic strain, rotation, and Cauchy stress fields
around the inclusion, that vary with position vector \( x \). \( E, W, \) and \( \Sigma \) are the far-
field elastic strain, rotation, and Cauchy stress fields in the embedding medium.
\( C^{\text{in}} \) and \( C^{\text{M}} \) are the 4th order elastic stiffness tensors of the inclusion and the
embedding medium, respectively.
Figure 1.3. A schematic diagram to illustrate MOPLA (a) A crustal deformation zone of characteristic length $D$ with boundary conditions fluctuating at a scale of $\lambda$. (b) The macroscale deformation of the zone at an arbitrary point $X$ is defined in terms of a Representative Volume element (RVE), centered at $X$ and with a characteristic length $D$. $D \ll D$ and $D \ll \lambda$. (c) The RVE contains a representative assemblage of all rheologically distinct elements (RDEs). The mean size of RDEs is denoted by $d$ ($d\ll D$). The local fields are defined with each individual RDEs.
(d) Each RDE is regarded as an ellipsoidal Eshelby inclusion embedded in a hypothetical Homogeneous Equivalent Medium (HEM), whose rheological property is obtained by self-consistent homogenization from the rheological properties of all constituent elements contained in the RVE. The local fields in an RDE, also known as partitioned fields, govern the fabric development at local scale such as (e) fabric elements in outcrops (f) the microscopic shape fabric elements or (g) the crystallographic fabric within the RDE. The characteristic lengths of such fabric elements are denoted by $\delta$ ($\delta \ll d$). The absolute size of the characteristic lengths used in the model and the scale gaps between them will depend on the specific nature of problem under consideration. (Modified after Jiang, 2014).
1.2 Thesis Outline

This thesis aims to understand the heterogeneous deformation of Earth’s lithosphere by applying the self-consistent Multi Order Power Law Approach (MOPLA, Jiang and Bentley, 2012; Jiang, 2014, 2016; Lu, 2020) to different geological examples. To achieve this objective, this thesis is divided into six chapters. Chapter 1 discusses the motivation and guiding philosophy behind the work. Chapters-2 presents computational methods needed to solve geological problems in this thesis, while Chapters-3, 4, and 5 respectively tackle the specific geological problem. Chapter-6 summarizes the contributions of this thesis and provides the way forward for future research. The key contributions in Chapters-2 to 5 are summarized below:

While viscous inclusion problems in an isotropic medium can be readily solved using quick solutions with quasi-analytical accuracy (Jiang, 2016), inclusion problems in anisotropic medium require numerically intensive computation using quadrature techniques. Qu et al. (2016) developed an optimal scheme for evaluating the mechanical field inside an inclusion embedded in a general anisotropic viscous medium. However, calculating the mechanical fields around the inclusion still remains a challenge (Jiang, 2016). Chapter-2 develops an open-source MATLAB code for evaluating mechanical fields around a 3-D viscous inclusion embedded in a general anisotropic viscous medium. As a demonstration of its use, deviatoric stress and pressure fields are numerically evaluated around a 3-D viscous inclusion embedded in a planar anisotropic viscous medium.

For decades, geologists have understood the c-axis fabrics using the single-scale simulations of the Taylor-Bishop-Hill model (e.g., Lister et al., 1979) or VPSC model (Lebensohn and Tome, 1993). No quantitative approach to study the influence of partitioned flow on c-axis fabrics is available. Chapter-2 develops a MATLAB implementation that couples MOPLA with the VPSC model for c-axis fabric development to study the influence of flow partitioning on c-axis fabrics.

Pressure in and around a heterogeneous rock element in Earth’s lithosphere undergoing deformation is expected to deviate from its ambient value generally. Despite decades of
research, the significance of this pressure deviation is still debated. Varied and contradictory results have been obtained in previous models, which strongly depend on boundary conditions, rheology, and loading conditions considered. Chapter-3 investigates this pressure deviation in rheologically heterogeneous rocks.

Quartz c-axis fabrics in natural mylonites can vary to such an extent that they apparently give opposite senses of shear within a single thin section. Many hypotheses have been invoked to explain this. Chapter-4 investigates this quartz c-axis fabric variation using the multiscale approach coupling MOPLA and VPSC developed in Chapter-2 and identifies partitioned flow to be responsible for observed c-axis fabric variation.

Flanking structures are deflections in linear or planar fabric elements around a cross-cutting element such as a dyke or a vein and are useful tools for inferring kinematic information from rocks such as shear sense and finite strains. Previous simulations of flanking structures are limited to specific cases of frictionless slip surface (assuming the cutting element as inviscid material), limited cutting element’s shape and orientation, 2-D flows, and low finite strains. However, in a natural setting, the rheological properties of the cutting element mainly its strength, shape, and orientation can be highly variable. Common examples include flanking structures associated with a cross-cutting dyke or a mineral inclusion. Chapter-2 develops a new approach of simulating flanking structures around 3-D cutting elements of any rheological contrast with the embedding medium, varied geometry, and for deformation up to high finite strains. Chapter-5 uses this approach to simulate 3-D flanking structures and demonstrate how flanking structures may vary with cutting element’s rheological properties, shape, and orientation. A reverse-dynamic model is further developed to extract quantitative kinematic information such as kinematic vorticity number, finite strain, and viscosity contrast of the cutting element to the surrounding medium from some natural flanking structures.
1.3 References


2 Computational methods

2.1 Introduction

Earth’s lithosphere may record various types of structural features and fabric patterns due to tectonic deformation. Such structures may range from a c-axis fabric at the thin section scale to a structural feature such as a fold or fault at the outcrop scale, to the tectonic scale feature such as a ductile shear zone (e.g., Twiss and Moores, 1992; Pollard and Fletcher, 2005). To understand the deformation processes responsible for the formation of these structures and thereby understand the dynamics of Earth’s lithosphere, structural geologists have mainly used the theoretical framework of classical continuum mechanics (Jiang 2014). However, Earth’s lithosphere is heterogeneous at different scales of observation and composed of rheologically distinct elements (RDEs), leading to flow field partitioning (Lister and Williams, 1983). The classical continuum mechanics approach, which is limited to a single scale, cannot relate the thin-section to outcrop-scale structures in rocks to the tectonic scale deformation boundary conditions. Many geologists have recognized this problem and realized that capturing the influence of flow partitioning on rock records is fundamental in relating the thin-section to outcrop-scale structural features to the tectonic scale deformation (e.g., Lister and Williams, 1983; Jiang 1994a, b; Jiang and White, 1995; Jiang and Williams, 1999; Goodwin and Tikoff, 2002; Jones et al., 2005). Clearly, a multiscale approach is required for this purpose.

Recently, a micromechanics-based self-consistent Multi Order Power-Law Approach (MOPLA, Jiang and Bentley, 2012; Jiang, 2014, 2016) has been developed to address the issue of flow partitioning in rocks and simulate the multiscale deformation of Earth’s lithosphere. The theory and algorithms of MOPLA are well documented in Jiang (2014, 2016), and related computations are implemented in Mathcad (Jiang, 2014) and MATLAB (Qu et al., 2016; Lu, 2020). However, for applications to specific geological problems addressed in this thesis, certain refinements are required in the numerical implementation. In this work, I present new algorithms along with the MATLAB
implementations to apply MOPLA to specific geological problems addresses in this thesis such as pressure variation around a heterogeneous rock element in a general anisotropic medium, development of c-axis fabrics under partitioned flow, and simulating flanking structures.

To facilitate the description of the new implementation, I first present the backbone theory of MOPLA and summarize the key equations. Then, I discuss new implementations developed for respective geological problems along with examples to demonstrate the use of the MATLAB package. A brief description of MATLAB code and download link is given in the Appendix.

2.2 The Eshelby inclusion problem and significant equations

Fig 2.1 illustrates the Eshelby inclusion problem that forms the backbone theory of MOPLA. The general Eshelby formalism for a viscous ellipsoidal inclusion (Lebensohn et al., 1998; Jiang, 2016) relates the local fields inside (strain rate \( \varepsilon \), vorticity \( w \), deviatoric stress \( \sigma \), and pressure \( p \)) and around (strain rate \( \varepsilon(x) \), vorticity \( w(x) \), deviatoric stress \( \sigma(x) \), and pressure \( p(x) \)) the inclusion to their far-field counterparts in the embedding medium (namely, the strain rate \( E \), vorticity \( W \), deviatoric stress \( \Sigma \), and pressure \( P \)). Eshelby (1957) found that the mechanical fields inside the ellipsoidal inclusion (interior fields) are constant while the fields around and in the close vicinity of the inclusion (exterior fields) vary spatially with the position vector \( x \).
The following set of equations summarizes the solutions to the interior fields (Jiang, 2016, Eq. 12 there):

\[
\begin{align*}
\varepsilon &= \left[ J^d - S^{-1} \right]^{-1} : C^{-1} : (\sigma - \Sigma) + E \quad (2.1a) \\
\omega &= \Pi : S^{-1} : (\varepsilon - E) + W \quad (2.1b) \\
p &= \Lambda : C : S^{-1} : (\varepsilon - E) + P \quad (2.1c)
\end{align*}
\]

where the sign “:\:“ stands for double-index contraction of two tensors. \(C\) is the 4th-order viscous stiffness (viscosity) of the matrix material. \(S\) and \(\Pi\) are respectively the 4th-order symmetric and anti-symmetric Eshelby tensors for incompressible viscous materials and they are related to the inclusion shape and \(C\). \(\Lambda\) is a second-order auxiliary tensor also.

Figure 2.1 An illustration of Eshelby inclusion problem of an ellipsoidal viscous inclusion embedded in an infinite homogeneous viscous medium. \(\varepsilon\), \(\omega\), \(\sigma\) and \(p\) are the uniform strain rate, vorticity, deviatoric stress and pressure fields inside the inclusion. \(\varepsilon(x), \omega(x), \sigma(x)\) and \(p(x)\) are the strain rate, vorticity, deviatoric stress and pressure fields around the inclusion, that vary with position vector \(x\). \(E\), \(W\), \(\Sigma\) and \(P\) are the far-field strain rate, vorticity, deviatoric stress and pressure fields in the embedding medium. \(C^{in}\) and \(C\) are the 4th order viscous stiffness tensors of the inclusion and the embedding medium, respectively.
calculated from inclusion shape and $\mathbf{C}$. $\mathbf{J}^d$ is the 4th-order deviatoric identity tensor used by Jiang (2016, 2014) for incompressible materials. It is defined in terms of Kronecker delta ($\delta_{ij} = 1$ for $i = j$ and $\delta_{ij} = 0$ for $i \neq j$) as:

\[ J_{ijkl} = \frac{1}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) - \frac{1}{3} \delta_{ij} \delta_{kl}. \]

The following set of equations summarizes the solutions to the exterior fields (Jiang, 2016, Eq13 there):

\[
\begin{align*}
\mathbf{e}(\mathbf{x}) & = \mathbf{E} + \mathbf{S}^E(\mathbf{x}) : \mathbf{S}^{-1} : (\mathbf{e} - \mathbf{E}) \quad (2.2a) \\
\mathbf{w}(\mathbf{x}) & = \mathbf{W} + \mathbf{\Pi}^E(\mathbf{x}) : \mathbf{S}^{-1} : (\mathbf{e} - \mathbf{E}) \quad (2.2b) \\
p(\mathbf{x}) & = P + \mathbf{\Lambda}^E(\mathbf{x}) : \mathbf{C} : \mathbf{S}^{-1} : (\mathbf{e} - \mathbf{E}) \quad (2.2c)
\end{align*}
\]

where $\mathbf{S}^E(\mathbf{x})$ and $\mathbf{\Pi}^E(\mathbf{x})$ are 4th-order symmetric Eshelby tensor for exterior field related to the inclusion shape, position vector, and the medium’s $\mathbf{C}$. $\mathbf{\Lambda}^E(\mathbf{x})$ is a second-order auxiliary tensor for external pressure field to be calculated from inclusion shape, position vector and $\mathbf{C}$.

For geological timescales (~Myr), rocks can be reasonably assumed to be viscous incompressible materials. Any rheologically distinct element (RDE) in Earth’s lithosphere can be regarded as an ellipsoidal Eshelby inclusion embedded in a macroscale medium. The rheology of the latter is approximated by a hypothetical homogeneous-equivalent medium (HEM) (Lebensohn and Tomé, 1993; Molinari et al., 1987) and obtained using a self-consistent homogenization approach that involves volume-weighted averaging the rheologies of the constituent RDEs. The Eqs. 2.1 and 2.2 referred to as partitioning equations thus describe the mechanical interactions between the RDE with the hypothetical HEM. The partitioning equations were derived for linear viscous materials only. For non-linear power-law viscous materials like rocks (Kohlstedt et al., 1995), there are no such exact solutions. One has to use a linearization approach (Lebensohn and Tome, 1993; Jiang, 2016) to extend these solutions to non-linear viscous materials. In this case, a linearized viscosity such as a tangent viscosity (e.g., Jiang and Bentley, 2012) is used in these equations.
Depending on the nature of the problem, an RDE can be any rheologically heterogeneous rock unit such as an eclogite lense embedded in a gneiss, a ductile shear zone in the lithosphere, quartz domains in heterogeneous shear zones, or any cross-cutting element such as a dyke or vein. The partitioning equations allow the evaluation of mechanical fields inside (strain rate $\varepsilon$, vorticity $w$, deviatoric stress $\sigma$, and pressure $p$ fields) and around (strain rate $\varepsilon(x)$, vorticity $w(x)$, deviatoric stress $\sigma(x)$, and pressure $p(x)$) the RDE which can then be utilized for solving specific problems. For example, the pressure fields in and around the rock unit can be used to estimate the order of magnitude of pressure deviations in Earth’s lithosphere due to tectonic deformation. Strain rate and vorticity fields within the quartz domains in heterogeneous shear zones can be used to simulate the development of c-axis fabrics. Strain rate and vorticity fields around a cross-cutting element such as a dyke can be used to simulate the displacement of planar or linear marker elements (also known as flanking structures) surrounding the cutting element.

The assumptions of ellipsoids for RDEs may introduce some uncertainties in the actual mechanical fields. The Eshelby solutions for ellipsoidal inclusions represent averaged mechanical fields in the RDE. For convex-shaped RDEs, the actual flow field variation in the element is small relative to the averaged field. Where the RDE is more irregularly shaped, mechanical fields may vary more significantly from the calculated average fields. For situations where shape effect is important, one has to consider Eshelby’s problem for non-ellipsoidal inclusions (e.g., Zou et al., 2010). For geological problems addressed in this thesis, RDEs are mainly convex bodies and can be reasonably treated as ellipsoids of varied shapes. An eclogite lense or a quartz domain can be represented by a triaxial-shaped ellipsoid while a ductile shear zone, a dyke, or a vein can be represented by a highly flattened ellipsoid. The Eshelby solutions provide good approximations to actual mechanical fields in these RDEs.

The use of HEM means that high-order local interactions are ignored, and a mean-field theory is applied. More complicated formulation and much more computation resources are needed to consider high-order local interactions. However, texture modeling of polycrystals has shown that considering high-order interactions does not lead to
significant changes in the modeled texture. This can be regarded as evidence that the mean-field approach, as used in this thesis, captures the first-order significant physics of the problem.

2.3 Exterior Eshelby solution in general anisotropic medium

Jiang (2016) simplified the Eqs. 2.1 and 2.2 above for the cases of inclusions embedded in an isotropic viscous medium and derived quick solutions with quasi-analytical accuracy. However, there are no such solutions for inclusions in a general anisotropic medium, which is more relevant to the geological materials (Ran et al., 2019). In such a case, one has to numerically evaluate the Eshelby tensors using standard quadrature techniques, which is computationally intensive. Recently, Qu et al. (2016) has developed an optimal scheme for numerically evaluating the Eshelby tensors $S$, $\Pi$, and $\Lambda$, and hence respective interior fields using Eq. 2.1 above. However, numerically evaluating the Eshelby tensors for exterior fields, namely $S^E(x)$, $\Pi^E(x)$, and $\Lambda^E(x)$, remains a challenge (Jiang, 2016). In this section, I provide a new implementation based on MATLAB vectorization to efficiently evaluate the exterior Eshelby tensors $S^E(x)$, $\Pi^E(x)$, and $\Lambda^E(x)$ which can then be used to evaluate respective exterior fields using Eq. 2.2 above. These solutions have wide applications in studying the heterogeneous deformation in anisotropic rocks.

The two Eshelby tensors $S^E(x)$ and $\Pi^E(x)$ can be further defined in terms of an auxiliary fourth-order tensor $T^E(x)$ as $S^E(x) = J^d : T^E(x) : C$ and $\Pi^E(x) = J^a : T^E(x) : C$, where $J^d$ is the 4th-order deviatoric identity tensor as defined above, and $J^a$ is the 4th-order anti-symmetric identity tensor defined as: $J^a_{ijkl} = \frac{1}{2} (\delta_{il} \delta_{kj} - \delta_{ik} \delta_{jl})$.

The auxiliary tensors $\Lambda^E(x)$ and $T^E(x)$ are given by following expressions (Jiang, 2016, Eq.10 there):

$$\Lambda^E_j(x) = \int_{\partial \Omega} H_i(x - x') n_j(x') dS(x') \quad (2.2a)$$
where $H_i(x - x')$ is the Green function for pressure and $G_{ik,l}(x - x')$ is the derivative of the Green function for velocity (Lebensohn et al., 1998; Jiang, 2016) and the integrations are over the ellipsoid surface $S(x')$ with $n_j$ being plane-normal unit vector component of the area element $dS$ on the ellipsoid surface.

Green functions $G_{ij}(x, x')$ and $H_i(x, x')$ relate respectively, the velocity $u_i(x)$ and pressure $p(x)$ at the location $x$ due to a unit point force at the source location $x'$. For an infinite medium, $G_{ij}(x, x') = G_{ij}(x - x')$ and $H_i(x, x') = H_i(x - x')$. Note that for simplicity $G_{ij}(x - x')$ and $H_i(x - x')$ is written below as $G_{ij}(x)$ and $H_i(x)$ setting the source point at the origin. Jiang (2016) obtained the formal expressions for these incompressible Green functions and their derivatives for anisotropic materials (his Eq. 8a, b, c), which are summarized as follows:

\[
G_{ij}(x) = \frac{1}{4\pi^2r^2} \int_0^\pi \tilde{A}_{ij} d\psi 
\]

\[
H_i(x) = -\frac{1}{4\pi^2r^2} \int_0^\pi F_i d\psi
\]

\[
G_{ij,l}(x) = \frac{1}{4\pi^2r^2} \int_0^\pi \left( \hat{x}_i \tilde{A}_{ij} + z_l \hat{M}_{ij} \right) d\psi
\]

where $\psi$ is a polar angle in the plane perpendicular to $\hat{x}$ (Fig. 2.2). $r = |x|$, $\hat{x}_i = \frac{x_i}{r}$,

\[
F_i = \tilde{A}_{in} Y_{mn} \zeta_m + \left( \lambda \tilde{A}_{in} + \zeta_1 \zeta_m \right) \hat{x}_m,
\]

\[
\hat{M}_{ij} = \tilde{A}_{im} \tilde{A}_{jn} Y_{mn} + \left( \tilde{A}_{im} \zeta_j + \tilde{A}_{jn} \zeta_i \right) \hat{x}_m
\]
with \( \Upsilon_{\alpha\beta} = C_{\alpha\rho\beta\sigma}(z_p \hat{x}_q + z_q \hat{x}_p) \),

\[
\begin{pmatrix}
\hat{A} & \hat{q}
\end{pmatrix} = \begin{pmatrix}
A & z
\end{pmatrix}^{-1}
\begin{pmatrix}
\zeta
\hat{\lambda}
\end{pmatrix}
\]

where \( A \) is the Christoffel stiffness tensor (e.g., Barnett, 1972) given by \( A_{ik} = C_{ijl} z_j z_l \), and \( z \) is a unit vector in the plane normal to \( x \) and can be expressed in terms of two mutually orthogonal unit vectors (\( \alpha \) and \( \beta \)) on the \( \hat{x} \cdot z = 0 \) plane (Fig. 2.2). \( z = \cos \psi \alpha + \sin \psi \beta \). When \( \hat{x} \) is expressed in terms of spherical angles \( \theta \) and \( \phi \) as \( \hat{x} = \begin{pmatrix} \cos \theta \sin \phi \\ \sin \theta \sin \phi \\ \cos \phi \end{pmatrix} \), then \( \alpha = \begin{pmatrix} -\sin \theta \\ \cos \theta \\ 0 \end{pmatrix} \) and \( \beta = \begin{pmatrix} -\cos \theta \cos \phi \\ -\sin \theta \cos \phi \\ \sin \phi \end{pmatrix} \).

**Figure 2.2.** Stereographic projection showing how, for any given \( x \), unit vector \( z \) in the plane normal to the \( x \), can be expressed in terms of two mutually orthogonal unit vectors on the \( \hat{x} \cdot z = 0 \) plane by \( z = \cos \psi \alpha + \sin \psi \beta \) following Barnett (1972).

In essence, evaluation of pressure \( p(x) \) boils down to numerically evaluating \( \Lambda^E(x) \) (Eq. 2.2a) while evaluation of strain rate \( \varepsilon(x) \), vorticity \( w(x) \), and deviatoric stress (\( \sigma(x) = C : \varepsilon(x) \)) boils down to numerically evaluating \( T^E(x) \) (Eq. 2.2b).
2.3.1. Numerical evaluation of $\Lambda^E(x)$ and $T^E(x)$:

$\Lambda^E_i(x)$ can be expressed in terms of spherical angles by the following expression:

$$\Lambda^E_i(x) = a_1 a_2 a_3 \int_0^{2\pi} \left[ \int_0^\pi [f(x, \theta, \phi)]_y \sin \phi d\phi \right] d\theta$$  \hspace{1cm} (2.4a)

where $[f(x, \theta, \phi)]_y = \frac{H_i(x-x')}{a_j}$ with $x' = \left( a_1 \cos \theta \sin \phi \right) \left( a_2 \sin \theta \sin \phi \right) \left( a_3 \cos \phi \right)$ and $\xi = \left( \cos \theta \sin \phi \right) \left( \sin \theta \sin \phi \right) \left( \cos \phi \right)$.

Eq. 2.4a is evaluated in two steps: First, we evaluate $H_i(x-x')$ by solving the integral in Eq. 2.3b with $x$ replaced by $x-x'$. We use a Gaussian quadrature to evaluate this integral as follows:

$$H_i(x) = -\frac{1}{4\pi^2 r^2} \int_0^\pi F_i d\psi = -\frac{1}{4\pi^2 r^2} \sum_{j=1}^{n_\psi} w_j g(\psi_j)$$  \hspace{1cm} (2.4b)

where $w_j$ are the Gauss-Legendre weights and $\psi_j$ are the Gauss-Legendre grid nodes, $n_\psi$ is the number of nodes and $g(\psi_j)$ is $F_i$ evaluated for the respective nodes. In the second step, we use a product Gaussian quadrature as in Jiang (2013, 2014) to finally evaluate Eq.2.4a, using the following expression:

$$\Lambda^E_i(x) = a_1 a_2 a_3 \sum_{q=1}^n \sum_{p=1}^n w_p w_q [f(x, \theta_p, \phi_q)]_y \sin \phi_q$$  \hspace{1cm} (2.4c)

where $(\theta_p, \phi_q)$ are Gauss-Legendre grid nodes, $w_p$ are the Gauss-Legendre weights, and $n$ is the number of nodes and weights. The total number of grid nodes used in Eq. 2.4c is thus $n^2$.

$T^E_{ijkl}(x)$ can be expressed in terms of spherical angles by the following expression:

$$T^E_{ijkl}(x) = a_1 a_2 a_3 \int_0^{2\pi} \left[ \int_0^\pi [f(x, \theta, \phi)]_{ijkl} \sin \phi d\phi \right] d\theta$$  \hspace{1cm} (2.5a)
where \[ f(x, \theta, \phi) \] is evaluated with \[ x' = \begin{pmatrix} a_1 \cos \theta \sin \phi \\ a_2 \sin \theta \sin \phi \\ a_3 \cos \phi \end{pmatrix} \] and \[ \xi = \begin{pmatrix} \cos \theta \sin \phi \\ \sin \theta \sin \phi \\ \cos \phi \end{pmatrix} \].

Similar to Eq. 2.4a above, Eq. 2.5a is evaluated in two steps: First, we evaluate \( G_{ijk}(x-x') \) by solving the integral in Eq. 2.3c with \( x \) replaced by \( x-x' \). We use a Gaussian quadrature to evaluate this integral as follows:

\[
G_{ij,k}(x) = \frac{1}{4\pi^2 r^2} \int_0^\pi \left( -\hat{x}_i \hat{A}_j + z_i \hat{M}_j \right) d\psi = \frac{1}{4\pi^2 r^2} \sum_{k=1}^{n_{\psi}} w_k g(\psi_k)
\]

where \( w_k \) are the Gauss-Legendre weights and \( \psi_k \) are the Gauss-Legendre grid nodes, \( n_{\psi} \) is the number of nodes and \( g(\psi_k) \) is \( \left( -\hat{x}_i \hat{A}_j + z_i \hat{M}_j \right) \) evaluated for the respective nodes. Second, we use a product Gaussian quadrature as in Jiang (2013, 2014) to finally evaluate Eq. 2.5a, using the following expression:

\[
T_{ijkl}^E(x) = a_1 a_2 a_3 \sum_{q=1}^{n_w} \sum_{p=1}^{n_w} w_p w_q [f(x, \theta_p, \phi_q)]_{ijkl} \sin \phi_q
\]

where \( (\theta_p, \phi_q) \) are Gauss-Legendre grid nodes, \( w_p \) are the Gauss-Legendre weights, and \( n \) is the number of nodes and weights. The total number of grid nodes used in Eq. 2.5c is thus \( n^2 \).

The error associated with evaluating the integrals above (Eqs. 2.4, 2.5) is unknown a priori. One can get an error estimate as follows: prescribe a tolerance and evaluate the integral iteratively, starting with a lower node number and progressively increasing the node number until the output converges with prescribed tolerance. We note that exterior points closer to the inclusion-medium boundary require a greater number of Gaussian nodes for accurate evaluation under a prescribed tolerance. In our calculations for stress and pressure fields below, we hence vary the number of Gaussian nodes for stress and pressure field evaluation at an exterior point around the inclusion with respect to its position from the inclusion-medium boundary. When considering a large number of
exterior points (required for iso-surfaces and cross-sections below), we have utilized the parallel computing toolbox in MATLAB for further increase in computation speed.

2.3.2. Vectorization approach for evaluating $\mathbf{A}^E(x)$ and $\mathbf{T}^E(x)$

In numerically evaluating $\mathbf{A}^E(x)$ above, there are two numerical quadrature involved (Eq. 2.4b and c). The integrand $F_i$ in Eq. 2.4b is also a function of $\phi_q$ and $\theta_p$. Therefore, Eq. 2.4b needs to be evaluated $n^2$ times for $n^2$ nodes corresponding to $\theta_p, \phi_q$. If one solves Eqs. 2.4b and 2.4c as separate functions in MATLAB, the evaluation is computationally intensive. Instead, one can vectorize this process such that $H_i(x-x')$ is evaluated for all $n^2$ grid nodes at once rather than a separate evaluation for each grid node. For this, each element of the auxiliary tensor $\mathbf{A}^E(x)$ (i.e. $\Lambda^E_q(x)$) is evaluated as a $n^2 \times n_x$ matrix (Fig. 2.3) where $n^2$ is the total number of grid nodes for product Gaussian quadrature in Eqs. 2.4c, and $n_x$ is the number of nodes for Gaussian quadrature in Eqs. 2.4b. The weighted sum across matrix dimension corresponding to $n_x$ solves first integral while the weighted sum across matrix dimension corresponding to $n^2$ solves the second integral.
Similarly, in numerically evaluating \( E^T \) above, there are two numerical quadratures involved (Eq. 2.5b and c). The integrand \( \hat{l}_{ij} \) is also a function of \( \phi \) and \( \theta \).

Therefore, Eq. 2.5b needs to be evaluated \( n^2 \) times for \( n^2 \) nodes corresponding to \( \theta, \phi \).

If one solves 2.5b and 2.5c as separate functions in MATLAB, the evaluation is computationally intensive. Instead, one can vectorize this process such that \( G_{y,i} (x - x') \) is evaluated for all \( n^2 \) grid nodes at once rather than a separate evaluation for each grid node. For this, each element of the auxiliary tensor \( T^E(x) \) (i.e. \( T_{ijkl}^E(x) \)) is evaluated as a \( n^2 \times n_\psi \) matrix (Fig. 2.3) where \( n^2 \) is the total number of grid nodes for product Gaussian quadrature in Eqs. 2.5c, and \( n_\psi \) is the number of nodes for Gaussian quadrature in Eqs.

Figure 2.3. A block diagram to represent each element of auxiliary tensors (\( \Lambda_{ij}^E(x) \) or \( T_{ijkl}^E(x) \)) evaluated as a \( n^2 \times n_\psi \) matrix. Weighted sums across the two dimensions of the matrix solves the two integrals (Eqs. 2.4b, c, 2.5b, c in the text).

Each element of the Auxiliary tensors, \( T_{ijkl}^E(x) \) and \( \Lambda_{ij}^E(x) \) evaluated as \( n^2 \times n_\psi \) matrix illustrated below.
2.5b. The weighted sum across matrix dimension corresponding to $n_\varphi$ solves first integral while the weighted sum across matrix dimension corresponding to $n^2$ solves the second integral.

2.3.3. Code validation and example problem

A brief description of the MATLAB code is provided in Appendix A. Here, I consider an example problem of an isotropic inclusion embedded in a linear viscous anisotropic medium. From Eqs.2.2, it is clear that the evaluation of exterior fields is independent of inclusion’s viscous stiffness tensor $C^\text{in}$. Hence, in this work we consider a simple case of isotropic inclusion with $C^\text{in} = 2\eta\mathbf{J}^d$, where $\eta$ is inclusion’s viscosity. Our formulation can be applied to anisotropic inclusions by simply defining a suitable $C^\text{in}$ (e.g., Chen et al., 2014). Although there can be different kinds of mechanical anisotropy in a system (e.g., Mura, 1987), we use the case of planar anisotropy, which is relevant to foliated rocks (e.g., Fletcher, 2009; Johnson and Fletcher, 1994, Jiang, 2016). Any general anisotropic medium can be considered in the formulation if required (e.g., Fig. 8 of Jiang and Bhandari, 2018).

The rheology of the planar anisotropic medium can be characterized by two distinct viscosities: $\eta_n$, the normal viscosity for the resistance to layering parallel shortening or extension, and $\eta_s$ the shear viscosity measuring the resistance to layering parallel shear (e.g., Jiang, 2016; Fletcher, 2009). The strength of anisotropy is measured by the ratio $m$ of $\eta_n$ to $\eta_s$. For foliated and layered rocks, $m$ is generally $> 1$ (Treagus, 2003).

The rheological contrasts between the isotropic inclusion and medium can be defined by the following two parameters: the ratio, $r$, between the viscosity of the inclusion to $\eta_n$ and $m$. Fig. 2.4 presents the geometry of the far-field flow, inclusion, and the plane of anisotropy of the embedding medium.
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The inclusion’s shape is given by its three semi-axes: \( a_1 \geq a_2 \geq a_3 \). Since our purpose here is to benchmark the code, we use a far-field pure shear flow and let \( a_i \) align parallel to the \( Z \)-axis, \( a_2 \) parallel to the \( X \)-axis, and \( a_3 \) parallel to the \( Y \)-axis. More complex 3-D flows and general 3-D orientations defined by spherical angles (e.g., Jiang, 2007, Qu et al., 2016; Lu, 2020) can be assigned in the code if required.

As there are no analytical solutions available for exterior mechanical fields in anisotropic media, we benchmark our code against the isotropic viscous inclusion solutions with quasi-analytical accuracy (Jiang, 2016). This situation is the special case of planar anisotropic medium when \( m = 1 \). Fig. 2.5 compares pressure (Figs.2.5a, b) and stress fields (Figs.2.5c, d) for some exterior points along \( X \) and \( Y \) axes using isotropic solutions (Jiang, 2016) and numerical solutions with code developed in this work. The inclusion is rheologically stronger than the medium with \( r = 10 \). The squares are values evaluated from the isotropic solutions whereas the circles are values evaluated from the numerical solutions in this work. The coinciding plots validate our code. Since the Eshelby solutions are scale-independent, one can apply these solutions for any absolute length scale with a given aspect ratio of the inclusion. Note that since deviatoric stress \( \sigma(x) \) is a second-order tensor and has 6 independent components, we have plotted its second invariant, given by \( \sigma_{ij}(x) = \sqrt{\frac{1}{2} \sigma(x)_{ij} \sigma(x)_{ij}} \) for validation of our code.
Figure 2.5 Pressure and deviatoric stress fields at some exterior points around inclusions of different shapes (a) Pressure fields at exterior points along X-axis (b) Pressure fields at exterior points along Y-axis (c) Stress invariant fields at exterior points along X-axis (b) Stress invariant fields at exterior points along Y-axis. The squares are respective fields evaluated using the isotropic solutions of Jiang (2016) while the circles are respective fields evaluated using the code developed in this work.
Fig. 2.6 shows improvement in computation speed due to vectorization of the code (See Appendix A for more details). The circles correspond to the time taken for the evaluation of exterior pressure fields using non-vectorized code while the squares correspond to the time taken for the evaluation of exterior pressure fields using vectorized code. The time taken using the vectorization approach is reduced by more than half as the number of Gaussian points is increased. As the plot for time vs Gaussian points is logarithmic, for the number of Gaussian points ~500, which is required for a highly flattened or elongated ellipsoid, the time difference between the vectorized code and non-vectorized code will be increased further.

![Figure 2.6 Plot of computation time for pressure field at an arbitrary exterior point coordinate (0,0,4) around an inclusion of aspect ratio 5:3:2, with respect to the number of Gaussian points. The circles are values evaluated using the non-vectorized code, while the squares are values evaluated using vectorized code.](image-url)
Fig 2.7 presents the full 3-D pressure fields in and around a strong inclusion ($r = 10$) with axial ratios $5:3:2$. Figs. 2.7a-c shows the 3-D pressure iso-surfaces and cross-sections for the inclusion in an isotropic medium ($m = 1$). Figs.2.7d-f are similar plots as in Figs. 2.7a-c but for a planar anisotropic medium with $m = 10$. Fig.2.8 presents the full 3-D stress invariant fields in and around a strong inclusion ($r = 10$) with axial ratios $5:3:2$. Figs. 2.8a-c shows the 3-D stress invariant iso-surfaces and cross-sections for the inclusion in an isotropic medium ($m = 1$). Figs. 2.8d-f are similar plots as in Figs. 2.8a-c but for a planar anisotropic medium with $m = 10$. The undulations of iso-surfaces in anisotropic media (Figs. 2.7d,2.8d) are due to the errors in numerical evaluation. The spatial variation of pressure and stress invariant fields around the inclusion (Figs. 2.7b,c,e,f, 2.8b,c,e,f) is similar in both isotropic and planar anisotropic systems. However, the maximum values of pressure, as well as stress invariant fields around the inclusions, are reduced in the planar anisotropic medium as compared to the isotropic medium cases.
Figure 2.7 3D pressure deviation fields related to a strong inclusion (viscosity ratio $r = 10$) with axial lengths 5:3:2) in an isotropic ($m=1$) medium (left column) and in a planar anisotropic ($m=10$) medium (right column) under pure shearing flow. (a): Plot of 3D iso-pressure surfaces $\tilde{p}/\Sigma_m = -0.3, 0, 0.3$ (in purple, green, and yellow, respectively) for the isotropic medium case. (b) and (c): Respectively, the XY and XZ cross sections of the pressure fields for the isotropic HEM case. (d)-(f): Corresponding plots to (a)-(c) for the planar anisotropic HEM case ($m=10$). Compared to the isotropic HEM situation, the pressure fields related to the RDE in the anisotropic HEM situation are universally reduced. Note the (a)-(c) set of plots and the (d)-(f) set of plots use independent scale bars for pressure strength.
Figure 2.8 3D stress invariant fields related to a strong inclusion (viscosity ratio $r = 10$) with axial lengths 5:3:2) in an isotropic ($m=1$) medium (left column) and in a planar anisotropic ($m=10$) medium (right column) under pure shearing flow.

(a): Plot of 3D iso-stress invariant surfaces $\sigma_{ij}(x)/\Sigma_{jj} = 0.8, 1, 1.2$ (in purple, green, and yellow, respectively) for the isotropic medium.
2.4 C-axis fabric development under partitioned flow

C-axis fabrics in mineral aggregates of quartz, calcite, clinopyroxene, and olivine from the Earth’s lithosphere provides useful information on rock deformation such as deformation mechanism (e.g., Schmid and Casey, 1986; Stipp et al., 2002; Kepler, 2018), temperature (e.g., Faleiros et al., 2016; Law, 2014), and flow kinematics (e.g., Lister and Hobbs, 1980; Price, 1985; Simpson and Schmid, 1983; Bascou et al., 2002; Bestmann et al., 2000, 2002) of the ductile shear zones. To better understand the development of c-axis fabrics and effectively extract such information, several numerical modeling investigations (e.g., Etchecopar, 1977; Etchecopar and Vassuer, 1987; Lister and Williams, 1979; Lister et al., 1978; Lister and Paterson, 1979; Lister and Hobbs, 1980; Molinari, 1987; Lebensohn and Tome, 1993; Wenk et al., 1989; Wenk, 1999; Morales et al., 2011; Nie and Shan, 2014) have been carried out. A brief history of key numerical developments is summarized as follows: Etchecopar (1977) and Etchecopar and Vassuer (1987) developed a purely geometrical approach, where they regarded polycrystalline aggregate as a collection of 2-D polygonal cells (in Etchecopar, 1977) or 3-D polyhedral cells (in Etchecopar and Vassuer, 1987). These cells were assumed to deform using a small number (<5) of independent slip systems. The crystal aggregate was deformed such that the gaps and overlaps between the grains were minimized. Due to the geometric nature of the model, the relative activity of slip systems could not be assigned. This made it hard to relate active slip systems in the modeled c-axis fabrics to natural examples. Lister and coworkers (e.g., Lister et al., 1978; Lister and Williams, 1979; Lister and Paterson, 1979; Lister and Hobbs 1980) were the first to develop an intensive numerical approach that captured some aspects of the underlying microscopic physical processes responsible for c-axis fabric formation. They applied the Taylor-Bishop-Hill analysis...
(Taylor, 1938; Bishop and Hill, 1951; Bishop, 1953, 1954), where a polycrystalline aggregate was assumed to deform homogeneously with uniform strain in all the grains. This uniform strain was accommodated by intracrystalline slip on various slip systems, that followed a rigid-plastic behavior. The slip systems were chosen based on a plastic work criterion (Bishop and Hill, 1951). Activation of up to five independent slip systems was necessary to achieve a strain increment. Despite its limitations of uniform strain and rigid plastic behavior, the modeled fabric successfully resembled some naturally observed c-axis fabrics. In subsequent years, a Viscoplastic-Self-Consistent (VPSC) approach (e.g., Molinari, 1987; Lebensohn and Tome, 1993) has been developed that considers the mechanical interaction of grains with the surrounding matrix instead of assuming homogeneous strain as in Taylor-Bishop-Hill analysis. The deformation within the grains is achieved by intracrystalline slip-on slip systems that follow a rate-sensitive viscoplastic behavior. Due to its more realistic assumptions, the VPSC approach has been widely applied by material scientists and geologists to simulate c-axis fabrics of various rock-forming minerals (e.g., Wenk et al., 1989; Wenk, 1999; Bascou et al., 2002; Morales et al., 2011; Nie and Shan, 2014) and has successfully reproduced natural and experimental c-axis fabrics. For a comprehensive review of the VPSC application, the reader is referred to the work of Wenk (1999).

Despite the success of the Taylor-Bishop-Hill analysis and VPSC approach, a fundamental assumption remains in these modeling investigations that may cause problems in their application to the natural c-axis fabrics. All these numerical investigations are single-scale models in which c-axis fabrics are developed under a uniform flow. However, in the lithosphere, flow can vary from one rheologically distinct element (RDE) to another (with space) as well as within an RDE (with time). This flow within an RDE often referred to as partitioned flow (Lister and Williams, 1983; Jiang, 2014) can influence c-axis fabrics. Geologists have often resorted to the concept of flow partitioning to qualitatively explain c-axis fabric variation in rocks (e.g., Kilian et al., 2011; Peternell et al., 2010; Passchier, 1983). However, no quantitative method is available to study the effect of partitioned flow on the c-axis fabrics.
In this section, I present a MATLAB implementation that couples the VPSC model of Lebensohn and Tome (1993) with the self-consistent flow partitioning Multi-Order-Power-Law-Approach (MOPLA) of Jiang (2014, 2016) to simulate c-axis fabrics under partitioned flow. As a demonstration of its use, I have modeled quartz c-axis fabrics under partitioned flow. MATLAB scripts of the implementation can be downloaded from the GitHub repository link, provided in Appendix B.

2.4.1. Coupling VPSC with MOPLA

We use the thin section photomicrograph of Kilian et al. (2011) as an example (Fig. 2.9a) to illustrate our multiscale approach. We consider flow at two separate scales, a macroscale, and a microscale. A macroscale refers to a flow field defined in terms of a Representative Volume Element (RVE) that is about the size of the whole thin section. In such RVE, the rock consists of domains of quartz aggregates, feldspar aggregates, and mica-rich seams which shall be generally referred to as RDEs. The flow field in any one such RDE is distinct and differs from the macroscale flow. A microscale refers to such a flow field within an RDE, also called the partitioned flow field. For our example of quartz c-axis fabric development in this work, we specifically focus on the partitioned flow fields within RDEs of quartz aggregates (or quartz domains). Our approach can be applied to the c-axis fabrics of any other mineral aggregates occurring as heterogeneous domains in a similar RVE from a ductile shear zone.

We regard each quartz RDE as a heterogeneous ellipsoidal inclusion (an ellipsoidal inhomogeneity in the sense of Eshelby, 1959, 1957) embedded in the macroscale material (Fig. 2.9d). Although the latter is rheologically heterogeneous, in MOPLA it is represented by a homogeneous-equivalent medium (HEM) (e.g., Jiang, 2014; Lebensohn and Tomé, 1993) whose rheology is obtained self-consistently using homogenization from the rheological properties of all constituent elements contained in the RVE with which the macroscale flow is defined. The partitioning equations (Eq. 2.1a and 2.1b) describe the interaction between the RDE and HEM and relate the microscale and macroscale fields.
Figure 2.9: Illustration of the multiscale approach. (a) The thin section photomicrograph of a natural mylonite from Kilian et al. (2011) used as a model. (b) Sketch of (a). The thin section can be viewed as a 2D section of the representative volume element (RVE) for the shear zone material, which is composed of quartz domains, feldspar porphyroclasts, and mica seams in a fine-grained matrix. The quartz domains and feldspar clasts are referred to as Rheologically Distinct Elements (RDEs). We are concerned with partitioned flows in quartz RDEs in this paper. (c) Coordinate system to define the macroscale flow field used in modeling investigation. (d) Each quartz RDE is regarded as a heterogeneous Eshelby inclusion embedded in the composite shear zone material that is idealized as the Homogeneous Equivalent Matrix (HEM). Microscale fields (strain rate $\dot{\varepsilon}$, and vorticity $\omega$) are related to respective macroscale fields ($\mathbf{E}$ and $\mathbf{W}$) by partitioning equations, where $A$ is the strain rate partitioning tensor, $S$ and $\Pi$ are respectively the 4th-order symmetric and anti-symmetric Eshelby tensors (Jiang, 2014).
The rheologies of RDEs and HEM are generally anisotropic; the rheological contrast between any RDE and the HEM must be represented by a tensorial quantity. For simplicity, we assume that the quartz RDEs are always isotropic. The rheology of the HEM should ideally be obtained through self-consistent homogenization from the rheologies of its constituent RDEs. However, since the rheological properties of RDEs are not available, we consider two situations for the HEM. In the first, we assume that the HEM is also rheologically isotropic. In such a case, the rheological contrast between an RDE and the HEM is reduced to a scalar effective viscosity ratio \( r \) between the RDE to the HEM. In the second situation, we consider a HEM having a planar anisotropy which represents the foliation and layering commonly developed in mylonites. The rheology of such a HEM can be characterized by two distinct viscosities: \( \eta_n \), the normal viscosity for the resistance to layering parallel shortening or extension, and \( \eta_s \) the shear viscosity measuring the resistance to layering parallel shear (e.g., Jiang, 2016; Fletcher, 2009; Johnson and Fletcher, 1994). The strength of anisotropy is measured by the ratio \( m \) of \( \eta_n \) to \( \eta_s \). For foliated and layered rocks, \( m > 1 \) (Treagus, 2003). The rheological contrasts between the isotropic quartz RDE and HEM can be defined by the following two parameters: the ratio, \( r_{\text{eff}} \), between the viscosity of the RDE to \( \eta_n \) and \( m \). In such a case, the effective viscosity of the RDE is simply given by \( r_{\text{eff}} \eta_n \). Fig. 2.10 shows the geometric relation between the flow field and the plane of anisotropy. Macroscale flow is simple shear with shear plane parallel to X-Z plane.
Under a given macroscale flow, the numerical calculation using Eqs. 2.1a, b of the partitioned flow in a given RDE with initial shape, orientation, and relative viscosity are realized using MATLAB scripts available from the online GitHub repository (link provided in Appendix B). Once the partitioned flow in a quartz RDE is obtained from MOPLA, it is used as the input flow field for the simulation of the c-axis fabrics in that RDE. We use VPSC7 software (Lebensohn and Tomé, 2009) for Windows to simulate quartz c-axis fabrics. As the partitioned flow field in any given RDE changes with time as the RDE evolves in shape, orientation, and effective viscosity during deformation, a coupled computation between MOPLA and VPSC must be established. We export the partitioned flow field in an RDE, expressed as a velocity gradient tensor, to a data file at every prescribed strain increment of macroscale deformation until a set macroscale finite strain is reached. This data file is then used as input flow into the VPSC code, utilizing the VAR_VEL_GRAD subroutine of VPSC code (Lebensohn and Tomé, 2009). The VPSC output of the c-axis fabric data of the RDE is plotted using the MTEX toolbox (Bachmann et al., 2010).

2.4.2. MATLAB implementation

Figure 2.10: Geometric relation between the macroscale flow field and anisotropy plane in the planar anisotropic HEM.
Before running the MATLAB functions described below, it is required to add the MTEX toolbox folder to the MATLAB direction and launch the MTEX toolbox by running the “startup_mtex” in the MATLAB command window.

Main functions:

*Multi_Parameters_Iso_HEM.m*: This function couples MOPLA calculation for an RDE embedded in an isotropic HEM with the VPSC code. Its inputs are: $\Psi_k$: kinematic vorticity number to determine the flow, $r$: initial viscosity ratio of the RDE to the HEM. $a$: initial shape of the RDE, $\text{ang}$: initial orientation of the RDE given by spherical angles, $N_m$: Power-law stress exponent for the HEM, $N_c$: Power-law stress exponent for the RDE, $J_d$: Fourth order identity tensor, $b$: set of 6 orthonormal symmetric second-order base tensors required for obtaining inverse of any fourth-order tensor, and $\text{strI}$: finite strain intensity up to which the simulation needs to be run.

Its outputs are: “file_name.dat” file that contains partitioned flow field information to be used in VPSC code, “TEX_PH1.out” file that contains the information of the c-axis texture, C-axis fabrics plotted as MATLAB figure file.

*Multi_Parameters_Aniso_HEM.m*: This function couples MOPLA calculation for an RDE embedded in a planar anisotropic HEM with the VPSC code. Its inputs are: $\Psi_k$: kinematic vorticity number to determine the flow, $r$: initial viscosity ratio of the RDE to the HEM. $a$: initial shape of the RDE, $\text{ang}$: initial orientation of the RDE given by spherical angles, $\text{strI}$: finite strain intensity up to which the simulation needs to be run, and $m$: strength of planar anisotropy of HEM.

Its outputs are: “file_name.dat” file that contains partitioned flow field information to be used in VPSC code, “TEX_PH1.out” file that contains the information of the c-axis texture, C-axis fabrics plotted as MATLAB figure file.

Other files(sub-functions):
Editvpsc7input.m: This function edits the VPSC7.in file to change the input parameters of the VPSC code. Its input is the name of the file, containing the information regarding the partitioned flow.

PlotTexture_AB.m: This function plots the c-axis texture using the MTEX toolbox for MATLAB from the texture file obtained in VPSC code. Its input: “TEX_PH1.out” file that contains the information of the c-axis texture. Output: c-axis fabrics plotted as MATLAB figure file

Calc_Gamma.m: This function calculates the strain intensity of the flow at any given time step of the calculation. Its inputs are L: velocity gradient tensor of the flow, tincr: time increment used in the calculation, steps: number of steps in the calculation.

2.4.3. Example problem
To demonstrate the use of our multiscale approach in this section, we consider the example problem of the development of c-axis fabrics in quartz RDEs embedded in an isotropic HEM and a planar anisotropic HEM. For our demonstration purpose, we consider macroscale flow as simple-shearing. However, any general 3-D flow can be considered in the formulation, if required. In the coordinate system used in this investigation (Fig. 2.9c), the macroscale flow is defined by the following Eulerian velocity gradient tensor:

\[
L = \begin{pmatrix}
0 & \dot{\gamma} & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 
\end{pmatrix}
\]  

(2.6)

where \( \dot{\gamma} (\dot{\gamma} > 0) \) is the shear strain rate for the simple shearing component.

To consider a range of effective viscosities of the quartz RDEs, we let \( r \) and \( r_{\text{eff}} \) vary as .5, 2, 5, 10 in the isotropic HEM and planar anisotropic HEM respectively. Such choice is consistent with the microstructures of quartz aggregates (Fig. 2.9a) having convex shapes with surrounding matrix material wrapping around them, suggesting that quartz RDEs were rheologically stronger (\( r > 1 \)) than the ambient HEM. But \( r \) cannot be too high (e.g., \( r > 10 \)) because of power-law rheology or the quartz RDEs would behave like rigid clasts
(Jiang, 2007b; Xiang and Jiang, 2013) with no c-axis fabric formation. The situation of $r = 0.5$ is also considered here for comparison to show what the c-axis fabrics might be like if quartz RDEs were mechanically weaker than the ambient medium.

We consider RDEs of variable initial shapes and orientation to simulate the different quartz domains observed in Fig. 2.9a. The shape variation is covered by three reference initial shapes: prolate (5:1:1), oblate (5:5:1), and sphere (1:1:1). Initial triaxial-shaped RDEs with long and short semi-axial lengths fixed to 5 and 1 respectively and intermediate semi-axial lengths ranging from 2-4 are also considered. These initial RDEs will deform into various triaxial shapes possible in nature. The initial orientations of the RDEs are defined by spherical angles (Jiang, 2007b, 2007a) which are randomly assigned.

The relative activity of slip systems can be modulated in VPSC code by assigning relative critical resolved shear stress (CRSS) values. A lower CRSS corresponds to higher activity. For the demonstration purposes, we have used the quartz model with dominant basal\textsuperscript{a} slip system (Table 2.1) similar to ones used in previous work (e.g., Lister and Paterson, 1979; Morales et al., 2014; Wenk et al., 1989).

<table>
<thead>
<tr>
<th>Slip Systems</th>
<th>CRSS value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basal \textsuperscript{a} {0001} \langle \bar{1}2\bar{1}0 \rangle</td>
<td>1</td>
</tr>
<tr>
<td>Rhomb\textsuperscript{a} {10\bar{1}0} \langle \bar{1}2\bar{1}0 \rangle</td>
<td>5</td>
</tr>
<tr>
<td>Prismatic\textsuperscript{a} {10\bar{1}0} \langle \bar{1}2\bar{1}0 \rangle</td>
<td>5</td>
</tr>
<tr>
<td>Prismatic \textsuperscript{c} {10\bar{1}0} \langle 0001 \rangle</td>
<td>10</td>
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Table 2.1: Quartz model with the relative CRSS values used in VPSC simulation.

Fig. 2.11 presents c-axis fabrics from some selected cases of quartz RDEs embedded in isotropic HEM. Fig. 2.12 presents c-axis fabrics from some selected cases of quartz RDEs embedded in a planar anisotropic HEM. Our results can be summarized as follows: Modelled quartz c-axis fabrics comprise of c-axis girdles similar to ones obtained in
previous single-scale investigations (e.g., Morales et al., 2011). For quartz RDEs rheologically weaker than the ambient medium \((r < 1)\), the c-axis fabrics comprise either peripheral maxima or a girdle with peripheral maxima (Fig. 2.11 a-f, Fig. 2.12 a-f). For quartz RDEs rheologically stronger than the ambient medium \((r > 1)\), the c-axis fabrics comprise a c-axis girdle pattern with maxima at the periphery (Fig. 2.11 g-o, Fig. 2.12 g-o). The c-axis girdles are always antithetically-inclined (Figs. 2.11a, b, d, g, j, k, m, n, 2.12a, b, d, e, g, j, m) at low shear strain \((\gamma \sim 2-5)\) regardless of \(r, m, \) initial orientations and shapes of RDEs. The girdles rotate with bulk vorticity as \(\gamma\) increases (rows of Figs. 2.11 and 2.12) but do not pass the shear plane normal unless \(r \geq 2\) (Figs. 2.11h, i, l, o, 2.12i, l, o). If RDEs were weaker \((r = .5)\), c-axis girdles are close to normal (Figs. 2.11c, e, f, 2.12 c, f) to the shear plane even at high finite strains \((\gamma \sim 10-16)\).
<table>
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<tr>
<th>$r$ = 0.5, 5:1:1, (0,0)</th>
<th>$\gamma$ = 2</th>
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<tr>
<td>(a)</td>
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<tr>
<th>$r$ = 0.5, 5:3:1, (0,90,0)</th>
<th>$\gamma$ = 5</th>
<th>$\gamma$ = 10</th>
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<tr>
<td>(d)</td>
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<td>(g)</td>
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<th>$\gamma$ = 2</th>
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<tr>
<th>$r$ = 10, 5:2:1, (0,45,45)</th>
<th>$\gamma$ = 2</th>
<th>$\gamma$ = 5</th>
<th>$\gamma$ = 10</th>
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<td>(m)</td>
<td>(n)</td>
<td>(o)</td>
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</table>

Figure 2.11: C-axis fabrics in selected quartz RDEs in an isotropic HEM under simple shearing. (a)-(o) are the resultant c-axis fabrics developed. The first column presents the initial conditions for the RDEs [$r$ : viscosity ratio of the RDE to HEM, initial shape defined by semi-axes of the RDE ($a_1 : a_2 : a_3$, where $a_1 \geq a_2 \geq a_3$), and initial orientation given by spherical angles ($\theta_1, \Phi_1, \theta_2$) for general RDEs or ($\theta, \Phi$) for spheroidal RDEs]. Each row presents the results for the RDE as the macroscale strain increases. The c-axis densities are contoured in multiples of uniform distribution shown in the color bar.
Figure 2.12: C-axis fabrics in selected quartz RDEs in a HEM with planar anisotropy under simple shearing flow (a)-(o) are the resultant c-axis fabrics developed. The first column presents the initial conditions for the RDEs [$r$ - viscosity ratio of the RDE to HEM's $\eta$, initial shape defined by semi-axes of the RDE ($a_1 : a_2 : a_3$, where $a_1 \geq a_2 \geq a_3$), initial orientation given by spherical angles ($\theta_1$, $\Phi_1$, $\theta_2$) for general RDEs or ($\theta$, $\Phi$) for spheroidal RDEs, and anisotropic strength $m$]. Each row presents the results for the RDE as the macroscale strain increases. The c-axis densities are contoured in multiples of uniform distribution shown in the color bar.
2.5 Simulating 3-D flanking structures

Flanking structures are deflections in linear or planar fabric elements around any rheological heterogeneity, also known as the cross-cutting element, such as a fracture, vein, dyke, or a mineral inclusion (e.g., Passchier, 2001; Grasemann and Stuwe, 2001; Grasemann et al., 2003; Exner et al., 2004; Wiesmayr and Grasemann, 2005; Exner and Dabrowski, 2010; Grasemann et al., 2010; Mukherjee, 2014; Mukherjee and Koyi, 2013; Grasemann et al., 2016). They are potential tools for determining kinematic information from ductile shear zones of Earth’s lithosphere (e.g., Grasemann et al., 1999, Passchier et al., 2001, Passchier et al., 2005, Kocher and Mancktelow, 2005). The correct interpretation of a flanking structure is therefore essential for understanding regional tectonics (Grasemann et al., 2016). To understand the formation of these structures, several numerical investigations have been carried out over the last few years. These approaches can be summarized as follows: Grasemann and coauthors (Grasemann and Stuwe, 2001, Grasemann et al., 2003, Wiesmayr and Grasemann, 2005) were the first to numerically simulate flanking structures around a thin-slipping surface using a 2-D finite element modeling (FEM) approach. Their work demonstrated the formation of different kinds, namely, s- (synthetic slip), n- (no-slip), and a- (antithetic slip) type flanking structures as well as shear bands depending on the initial orientation of the slipping surface and flow type. Kocher and Mancktelow (2005) used a 2D solution for mechanical fields around an elliptical inclusion embedded in a viscous medium (Schmid and Podladchikov, 2003) to simulate flanking structures. This inclusion-based approach was semi-analytical and allowed deformation up to high finite strains. Mulchrone (2007) applied a similar 2-D analytical approach but with a different mathematical formulation for mechanical fields around elongated elliptical inclusion (Mulchrone and Walsh, 2006). They showed the variability in flanking structure formation depending on the cutting element’s initial orientation and viscosity and further used these solutions to determine the finite slip and curvature of any flanking structure. Exner and Dabrowski (2010) used the limiting case of Eshelby solution (Eshelby 1957,1959) for an elliptical crack to simulate flanking structures in 3D and showed that the 3-D model results in smaller offset across the cutting element than predicted with 2-D models.
Despite the success of these investigations in reproducing observed flanking structures, a few assumptions remain in these models that make it hard to apply them to natural scenarios. The majority of these models (e.g., Grasemann et al., 2003, 2005; Kocher and Mancktelow, 2005; Exner and Dabrowski, 2010) consider cutting elements as a weak frictionless slipping surface and simulate it as an inviscid material. However, in nature, the rheology of the cutting element such as a dyke or mineral inclusion can be more variable (e.g., Passchier, 2001; Mukherjee and Koyi, 2013) and form associated flanking structures of different types. The FEM-based approach of Grasemann et al., (2001) considered varying rheological contrast of the cutting element to the embedding medium but were limited to low finite strains (shear strain \( \gamma = 2 \)), 2-D flows, and limited cutting element aspect ratio (10:1). The models of Mulchrone (2007) were also limited to a very high aspect ratio of the ellipse (50:1). Besides, only the inclusion modeling approach by Exner and Dabrowski (2010) considered a 3-D flow and high finite strains. However, their solution is limited to a 2-D elliptical crack filled with inviscid material as mentioned above. To better understand the formation of natural 3-D flanking structures in ductile shear zones (e.g., Grasemann et al., 2011), it is highly critical to simulate flanking structures with more variable cutting element’s rheological contrast to the embedding medium, initial shapes, and orientations, 3-D flows and deformation up to high finite strains. None of the available approaches as discussed above can consider all of these influencing parameters that govern the development of a natural 3D flanking structure.

In this section, I present a new approach to model flanking structures in 3-D around any rheological heterogeneity using Exterior Eshelby solutions (Eqs. 2.1a, b, and 2.2a, b). The MATLAB implementation of this approach simulates flanking structures around a 3-D cutting element with varying rheological contrast with the medium, initial shape, and orientation, deformed under a far-field 3-D flow and up to high finite strains. For efficient calculations, a new method is developed for calculating velocity fields from the integration of respective velocity gradient fields around any 3-D cutting element. As a demonstration of its use, 3-D flanking structures are simulated around a cutting element subjected to far-field simple shear deformation. MATLAB code can be downloaded from the online GitHub repository (link provided in Appendix E).
2.5.1. A micromechanics-based model

Any rheological heterogeneity (or cutting element in terms of flanking structure terminology) can be regarded as a 3-D ellipsoidal Eshelby inclusion embedded in a viscous medium, and Eqs. 2.1a, b, and 2.2a, b allows the calculation of velocity gradient fields inside and around the heterogeneity respectively, given by Eulerian velocity gradient tensors, as follows:

\[ \mathbf{L} = \varepsilon + \mathbf{w} \quad (2.7a) \]

\[ \mathbf{L}(\mathbf{x}) = \varepsilon(\mathbf{x}) + \mathbf{w}(\mathbf{x}) \quad (2.7b) \]

As expected from Eshelby’s solution, the velocity gradient fields inside an inclusion are constant, while the velocity gradient fields outside the inclusion vary with the position vector. To simulate a flanking structure, which is merely a deflection of planar or linear marker elements surrounding the inclusion, one needs to obtain velocity fields at every time step of calculation of the rotating and deforming inclusion (e.g., Jiang, 2007) and then use it to evaluate the displacements of linear or planar marker elements at that step.

The velocity gradient tensor \( \mathbf{L} \) can be written as \( L_{ij} = \frac{\partial v_i}{\partial x_j} \), which can be rearranged to determine the velocity field as:

\[
\int_{v'_{i}}^{v_{i}} dv'_{i} = \int_{x',y',z'}^{x,y,z} L_{ij} dx_j
\]

where \( v'_i \) is the known velocity field at position vector \( x'^o \) which has coordinates \( (x'^o, y'^o, z'^o) \) and \( v_i \) is the velocity field to be calculated at position vector \( x \) which has coordinates \( (x, y, z) \). \( v_i \) and \( v'_i \) are the \( i \)th component of velocity vectors \( \mathbf{v} \) and \( \mathbf{v}^o \) respectively.

Assuming the center of the inclusion to be at rest and since \( \mathbf{L} \) is constant inside the inclusion, one can obtain the velocity field inside and at the inclusion surface as \( \mathbf{v} = \mathbf{Lx} \), where \( \mathbf{x} \) is the position vector of the point defined in inclusion’s coordinate system. For
any point outside the inclusion, velocity field needs to be calculated using Eq.2.8, which can be further written as:

\[ v_i = v_i^o + \int_{x^o}^{x} L_{ij} dx_j \]  \hspace{1cm} (2.9)

where \( x^o \) and \( v^o \) are the known position and velocity vectors respectively at any point on inclusion’s surface. The problem now boils down to evaluating the integral in Eq.2.9, which can be discretized in the interval \((x^o, x)\). Eq. 2.9 can then be rewritten as follows:

\[ v_i = v_i^o + \sum_{j=1}^{n} L_{ij}(x_j) \Delta x \]  \hspace{1cm} (2.10)

Where, \( n \) is the number of steps in which the interval \((x^o, x)\) is divided. \( \Delta x \) is the interval of each step and \( L_{ij}(x_j) \) is the velocity gradients evaluated at exterior points \( x_j \). (Note that repeated indices imply summation). Exterior Eshelby solutions for inclusion embedded in an isotropic medium are quick solutions with quasi-analytical accuracy (Jiang, 2016), therefore velocity gradient fields for all the exterior points can be quickly evaluated with high accuracy and efficiency.

Since there can be infinite paths along which the interval \((x^o, x)\) can be discretized for any exterior point \( x \), the most efficient way would be to find the shortest path for integration (Figs. 2.13b, 2.14b). We consider two cases. The first case is the special case when the far-field flow is a plane strain deformation with inclusion’s longest axis along the vorticity of the flow, and the marker surrounding the inclusion is a linear element along the 2-D cross-section (Fig. 2.13a). As the length of the longest axis goes to infinity, the situation becomes equivalent to the 2-D inclusion approach (e.g., Mulchrone, 2007). In this case, one can use the Cartesian-to Elliptical coordinate transformation and vice-versa (Sun et al., 2017, see Appendix C for more details) to discretize the integral in Eq.2.10. The exterior point \( x \) and the point \( x^o \) with known velocity are transformed into their respective Elliptic coordinates \((\xi, \eta)\) and \((\xi_o, \eta_o)\) respectively. The point \( x^o \) with known velocity is chosen such that \( \eta_o = \eta \). The interval \((x^o, x)\) can then be divided
into steps along the $\eta$ axis, such that the coordinate points of each interval are $(\epsilon_i, \eta)$ where $i = 1$ to $n$, $n$ being the number of steps (Fig. 2.13b). These points in elliptic coordinate systems are then converted back to Cartesian coordinates for evaluating the integral in Eq. 2.10.

Figure 2.13 Flanking structure model in plane-strain flows (a) Geometry of the inclusion with longest axis along $Z$-axis, and plane strain flow along $X$-$Y$ plane. CE is the cutting element (inclusion) while HE is the host element. (b) Coordinate lines of an elliptic coordinate system. The aspect ratio of the ellipse is the sectional aspect ratio of the ellipsoidal inclusion along $X$-$Y$ plane. The green line shows the path following $\eta$ axis along which interval $(x^e, x)$ is divided for solving the integral. See text for more details.

The second case is a general case and applies to any 3-D flow with planar or linear marker elements (Fig. 2.14a). In such a case, we use the Cartesian-to-Ellipsoidal coordinate transformation and vice-versa to discretize the integral in Eq. 2.10. The exterior point $x$ and the point $x^e$ with known velocity are transformed into their respective Ellipsoidal coordinates $(\varphi, \lambda, h)$ and $(\varphi^e, \lambda^e, h^e)$. The point $x^e$ with known
velocity is chosen such that $\varphi_o = \varphi, \lambda_o = \lambda$. The interval $(x^e, x^n)$ can then be divided into steps along the intersection of $h$ axis, such that the coordinate points of each interval are $(\varphi, \lambda, h_i)$ where $i = 1$ to $n$, $n$ being the number of steps (Fig. 2.14b). These points in ellipsoidal coordinate systems are then converted back to Cartesian coordinates for evaluating the integral in Eq. 2.10. Note that the Cartesian to Ellipsoidal coordinate system is not straightforward and requires numerical evaluation. We use a numerical approach following Eberly (2018), that calculates the foot point, that is the shortest distance from a given exterior point to the triaxial ellipsoid, using the Bisection method and then use analytical solutions (Panou and Korakitis, 2019) for calculating the respective $\varphi, \lambda, h$ coordinates (See Appendix D for more details).

**Figure 2.14.** Flanking structure model in a general 3-D flow (a) Inclusion (cutting element) surrounded by a planar marker (host element). Any general 3-D flow and orientation of cutting element can be considered in this case. (b) Inclusion coordinate system defined by x-y-z axes (respective semi-axes of the inclusion). For efficient evaluation of exterior velocity fields, Cartesian coordinate system is converted to Ellipsoidal coordinate system and vice versa. The green line shows the path following $h$ axis along which interval $(x^e, x^n)$ is divided for solving the integral. See text for more details.
2.5.2. Code validation and example problem

A brief description of the MATLAB code is provided in Appendix E. Here, we first validate our velocity field calculations with known examples of velocity fields surrounding circular and elliptical inclusions (e.g., Passchier et al., 2005). We then consider an example problem of simulating flanking structures around a cutting element subjected to a far-field deformation.

Fig. 2.15 presents the geometry of the far-field flow and cutting element. The cutting element’s initial shape is given by its three semi-axes: $a_1 \geq a_2 \geq a_3$ and any arbitrary initial orientation of the cutting element can be defined by spherical angles (Jiang, 2007). Since our purpose here is to demonstrate the use of our code, we use a far-field simple shearing flow. $a_1$ is aligned parallel to the Z-axis, and the initial orientation of the cutting element is given by angle $\theta$, between $a_2$ axis and the X coordinate axis. More complex 3-D flows and general 3-D orientations (e.g., Jiang, 2007, Qu et al., 2016; Lu, 2020) can be assigned in the code if required. The rheological contrast of the cutting element is defined by the ratio $r$ of inclusion’s viscosity to that of the embedding medium.

Figure 2.15: Geometry of the simple shearing flow and the cutting element. The flow is in the XY plane with shear strain rate axes parallel to the X-axis. The inclusion’s $a_1$-axis is parallel to Z and $\theta$ is the angle between $a_2$ and the X-axis.
Fig. 2.16 presents the velocity fields surrounding the ellipsoidal inclusions across the 2-D cross-section using the code developed in this work. Fig. 2.16a is the case of a cylinder while Fig. 2.16b is the case of an elliptical cylinder. The cylindrical inclusion is rheologically weaker than the ambient medium \((r = 0.02)\). This compares well with the published velocity fields cases of Passchier et al. (2005) (their Fig. 5b, 7e), based on 2-D elliptical inclusions, and hence validates our velocity fields calculation.

![Velocity flow fields around (a) a cylindrical cutting element (b) elliptic cylindrical cutting element with \(r = 0.02\). The elliptic cylinder has a sectional aspect ratio of 5:1. The arrows represent the velocity vectors.](image)

Figure 2.16: Velocity flow fields around (a) a cylindrical cutting element (b) elliptic cylindrical cutting element with \(r = 0.02\). The elliptic cylinder has a sectional aspect ratio of 5:1. The arrows represent the velocity vectors.

Fig. 2.17 presents a 3-D flanking structure around a cutting element with \(r = 10\), initial orientation \(\theta = 135^\circ\), and initial aspect ratio (10:5:1). The system is deformed up to a shear strain \(\gamma = 1\) (Fig. 2.17a) and 2.5 (Fig. 2.17b). The flanking structure in 3-D is comprised of the planar marker element (green) which gets deformed and folded in the vicinity of the cutting element, defined by the ellipsoidal inclusion (red). Based on the offset, the flanking structure can be classified as an s-type flanking structure with a synthetic offset along the cutting element.
Fig. 2.18 presents 2-D cross-sections of the flanking structures around a cutting element with $r = 10$, different initial orientations, given by $\theta = 135^\circ$, $90^\circ$ and $45^\circ$ respectively deformed up to a shear strain $\gamma = 2$. Depending on the initial orientation of the cutting element, all types of flanking structures, namely, s- (with synthetic slip), a- (with antithetic slip), and n- (with no-slip) type flanking structures can be formed.

Figure 2.17: 3-D flanking structure around a strong cutting element with viscosity ratio $r = 10$, initial sectional aspect ratio 5:1, and initial orientation given by $\theta = 135^\circ$. The flanking structure is an s-type flanking structure. The ellipsoidal inclusion (red) is the cutting element. The deformed surface (green) is the host element.
Figure 2.18: 2-D cross-sections of the flanking structures simulated around a strong cutting element with viscosity ratio $r = 10$, initial sectional aspect ratio 5:1, and initial orientation given by (a) $\theta = 45^\circ$ (b) $\theta = 90^\circ$ and (c) $\theta = 135^\circ$. Depending on the different initial orientations, ‘a’, ‘n’ and ‘s’ type offsets are developed in (a), (b) and (c) respectively.
2.6 Concluding remarks

This chapter provides refinements in the implementation of MOPLA required to solve specific geological problems in this thesis. We have developed a MATLAB code to numerically evaluate mechanical fields, namely, pressure, deviatoric stress, strain rate, and vorticity fields around a viscous ellipsoidal inclusion embedded in a general anisotropic medium subjected to a far-field deformation. These solutions have wide applications in modeling Earth’s heterogeneous lithosphere. The code has been benchmarked against the isotropic inclusion solutions of quasi-analytical accuracy (Jiang, 2016). The vectorized version of the code improves the computational speed up to 2-3 times. As a demonstration of its use, we have simulated deviatoric stress and pressure fields around a viscous inclusion embedded in a medium with planar anisotropy, which is common in foliated rocks. We found that the magnitudes of maximum deviatoric stress invariant and pressure fields in the anisotropic medium are reduced compared to the isotropic medium. The MATLAB code can be downloaded online from the GitHub repository link provided in Appendix A.

For our problem of investigating c-axis fabrics under partitioned flow, we have provided a MATLAB implementation coupling the VPSC code (Lebensohn and Tome, 1993; Lebensohn and Tome, 2010) with the MOPLA code (Jiang 2014, 2016, Qu et al., 2020; Lu 2020). As a demonstration of its use, we have modeled quartz c-axis fabrics under partitioned flow. Modeled quartz c-axis fabrics mainly comprise girdles similar to ones obtained in previous single-scale investigations. For quartz RDEs rheologically weaker than the ambient medium, the c-axis fabrics comprise a peripheral maximum. For quartz RDEs rheologically stronger than the ambient medium, the c-axis fabrics comprise a c-axis peripheral maximum with a girdle pattern. c-axis girdles can lie antithetically as well as synthetically to the shear plane depending on macroscale finite strain and quartz RDE’s rheology. MATLAB scripts of the implementation can be downloaded from the online GitHub repository link provided in Appendix B.

For the application of simulating flanking structures, we have developed a new algorithm along with MATLAB implementation that allows us to simulate 3-D flanking structures
around any cutting element with varying rheological contrast to the embedding medium, initial shapes, and orientation deformed under 3-D flow up to high finite strains. We use exterior Eshelby solutions to calculate velocity gradient fields surrounding the cutting element, which are then integrated to obtain respective velocity fields. We have developed an efficient method of velocity calculation from the velocity gradient fields, using the Ellipsoidal to Cartesian coordinate transformation (elliptic to Cartesian coordinate transformation for 2D cases) for the discretization of the involved integral. As a demonstration of its use, we simulate flanking structures in 3D around a rheologically strong cutting element. We show that depending on the initial orientation and cutting element’s viscosity, all types, namely s-, a-and n- types flanking structures can be formed around the cutting element. All the algorithms are implemented in a MATLAB code, which can be downloaded from the online GitHub repository link provided in Appendix E.
2.7 References


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Chapter 3

3 Pressure variations among rheologically heterogeneous elements in Earth’s lithosphere: A micromechanics investigation with comments on recent field reports of high-pressure minerals

3.1 Introduction

Pressure is an important variable in nearly all geological processes. Pressure estimates from mineral assemblages using various geothermobarometers (e.g., Spear, 1993) are routinely used as a proxy for the depth at which the assemblages were formed. This in turn is used to build geodynamic models for the geological process. However, it has been realized for many decades (Gerya, 2015; Mancktelow, 2008 and references therein) that tectonic deformation may cause the local pressure in a volume of rock to differ from the lithostatic pressure. This pressure difference has been called the ‘tectonic overpressure’ or ‘underpressure’, depending on whether the difference is positive or negative, in the literature. In this chapter, we shall use tectonic pressure deviation or simply pressure deviation to refer to the pressure difference caused by deformation because only pressure deviations from a mean ambient value are relevant in petrological records whereas the lithostatic pressure is unknown a priori. As established thermodynamic principles dictate that mineral assemblages are related to the total pressure, to convert geobarometric data to depth, it is critical to know how significant the error range may be due to the presence of possible tectonic pressure deviation. This includes the level of the tectonic pressure deviation, its variation in space from one geological unit to another at a given scale and across different scales, and the timespan an elevated pressure deviation (if generated) may be sustained. Although these problems have been tackled for over two decades through analytical (e.g., Mancktelow, 2008, 1995, 1993; Schmalholz et al., 2014b) and numerical modeling approaches (e.g., Burov et al., 2014; Li et al., 2010; Reuber et al., 2016), the results of these works are still controversial and inconsistent.

These works have shown quite clearly that the magnitude and variation of the tectonic pressure deviation are rather sensitive to the model geometry, boundary conditions,
rheologies, and rheological parameters assigned to the model elements. Simple models based on Jaeger (1969, p. 140-149) that have analytical solutions have been applied to natural transpressional zone deformation (Robin and Cruden, 1994) and extrusion or convergent channel systems (Mancktelow, 2008, 1995, 1993; Raimbourg and Kimura, 2008) and GPa-level pressure deviations have been predicted in the deforming zone (Mancktelow, 2008). However, these treatments regard the transpressional zone or the convergent channel as a tabular ‘deforming zone’ sandwiched between rigid or nearly rigid walls (country rocks) moving at a constant velocity relative to each other. The interface between the country rocks and the deforming zone is assumed to be fixed to material and is non-slippery. These assumptions lead to unrealistically strong mechanical interactions between the deforming zone and the country rocks and are, as we will show in this paper, responsible for the predicted GPa-level pressure deviations. Many 2D numerical models limited to elements of isotropic rheologies for large-scale collisional tectonic scenarios (e.g., Burg and Gerya, 2005; Burov et al., 2014; Li et al., 2010; Schmalholz et al., 2014a) have considered more reasonable boundary conditions. Differing results have been obtained with some getting ‘significant’ (> 20% of the lithostatic value) (e.g., Burg and Gerya, 2005; Schmalholz et al., 2014a) and others predicting ‘insignificant’ (< 20% of the lithostatic value) pressure deviation (e.g., Burov et al., 2014; Li et al., 2010). As each numerical modeling investigation uses a distinct computational procedure, it is not possible (e.g., Post and Votta, 2005) to identify how the inconsistency has arisen. It seems that the model results depend strongly on the loading condition and the choice of rheology and rheological parameters. The pressure deviation problem has also been analyzed using 2D inclusion solutions for isotropic Newtonian materials (Mancktelow 2008; Moulas, et al., 2014; Schmid and Podlachikov, 2003). Mancktelow (2008) concluded that the pressure deviations related to strong inclusions are of order 1-2 times the maximum shear stress the strong material can support. How the conclusion may be affected by power-law rheology, rheological anisotropy, and 3D inclusion deformation, which are all more relevant to natural deformation, is unknown.
In this paper, we apply a full mechanical approach – the generalized Eshelby’s inclusion solutions for power-law viscous materials (Jiang, 2016, 2014) to investigate the pressure deviation in natural deformation. This approach avoids unrealistic mechanical interactions caused by assumptions on rheological behaviors and boundary conditions and addresses the 3D deformation and anisotropic viscosity. Specifically, we regard the ductily-deforming rock masses undergoing metamorphism as a composite material made of rheologically distinct elements (RDEs). An RDE can represent any rheological heterogeneity, such as a distinct lithological unit or structural element like a ductile shear zone. We consider the long-term deformation with characteristic time scales on Ma, much greater than the viscous relaxation time (discussed later) so that elastic behaviors can be ignored. All RDEs and the composite material as a whole are assumed to be viscous. Supposing that a large representative volume of this ‘lithosphere material’ is subjected to a given macroscale deformation, we are concerned with how the pressure varies from one RDE to another and deviates from the bulk ambient pressure. To obtain the pressure deviation inside and around any RDE from the ambient pressure, we regard the RDE as an Eshelby inclusion embedded in the medium. The macroscale medium surrounding the RDE is rheologically heterogeneous, but in micromechanics, it is represented by a hypothetical homogeneous-equivalent medium (HEM) whose rheology is obtained self-consistently from the rheological properties of all constituent elements contained in a representative volume element (RVE) that embeds the RDE. Generalized Eshelby inclusion solutions for viscous power-law materials (Jiang, 2016, 2014, 2013) relate formally the local mechanical fields (including pressure) in and around the RDE to the macroscale mechanical fields. Pressure deviations inside and around the RDE can be computed with quasi-analytical accuracy using the partitioning equations from the Eshelby inclusion solutions. Because the formalism considers 3D deformation, non-linear viscous rheology, and rheological anisotropy, we can systematically investigate the pressure deviation as a function of these variables. As a thorough treatment of the generalized Eshelby solutions is given in Jiang (2016, 2014), only the partitioning equations used in this paper are presented in the following section.
3.2 Partitioning equations

The classical Eshelby inclusion/inhomogeneity problem is illustrated in Fig. 3.1. Initially, Eshelby (1959, 1957) solved for the elastic field inside and outside an isolated ellipsoidal domain. Eshelby called the domain an “inclusion” if it has identical elastic properties as the surrounding medium and an “inhomogeneity” if the domain has distinct elastic properties. For simplicity, we use “inclusion” to refer to any heterogeneous element in a composite material in this paper following Jiang (2016, 2014) unless a distinction must be made for clarity. Eshelby’s elegant point-force method and equivalent-inclusion approach have been extended to general anisotropic linear elastic materials as reviewed and summarized in Mura (1987) and general anisotropic linear viscous materials (see reviews of Jiang, 2016, 2014). The partitioning equations for the mechanical fields inside the inclusion are given in the following set (Jiang, 2016, Eqs.12 there):

\[
\begin{align*}
\tilde{\varepsilon} &= \left[ J^d - S^{-1} \right]^{-1} : C^{-1} : \tilde{\sigma} \quad (3.1a) \\
\tilde{w} &= \Pi : S^{-1} : \tilde{\varepsilon} \quad (3.1b) \\
\tilde{p} &= \Lambda : C : S^{-1} : \tilde{\varepsilon} \quad (3.1c)
\end{align*}
\]

In Eqs. 3.1, the sign “:” stands for double-index contraction of two tensors. The tilde above a quantity represents the deviation of that quantity from its far-field value, e.g., \( \tilde{p} = p - P \) (\( p \) and \( P \) stand for, respectively, the pressure in an element and the pressure in the far-field. Lowercase and uppercase symbols stands for local and far-field respectively). \( \tilde{\varepsilon}, \tilde{\sigma}, \tilde{w}, \) and \( \tilde{p} \) are the differences, respectively, in strain rate, deviatoric stress, vorticity, and pressure between the ellipsoidal inclusion and the far-field values in the embedding medium. \( C \) is the 4th-order viscous stiffness (viscosity) of the matrix material. \( S \) and \( \Pi \) are respectively the 4th-order symmetric and anti-symmetric Eshelby tensors for incompressible viscous materials and they are related to the inclusion shape and \( C \). \( \Lambda \) is a second-order tensor also calculated from inclusion shape and \( C \). \( J^d \) is the 4th-order deviatoric identity tensor used by Jiang (2016, 2014) for incompressible materials. It is defined in terms of Kronecker delta (\( \delta_{ij} = 1 \) for \( i = j \) and \( \delta_{ij} = 0 \) for \( i \neq j \))
as: \( J_{ijkl}^d = \frac{1}{2} (\delta_{ik} \delta_{jl} + \delta_{jk} \delta_{il}) - \frac{1}{3} \delta_{ij} \delta_{kl} \). The set of Eq. 3.1a, b, and c relates the mechanical fields inside an inclusion to the far-field mechanical fields and is called the interior solutions of the Eshelby problem. Specifically, Eq.3.1c gives the expression for the pressure deviation (from the ambient value) inside the inclusion.

The mechanical fields outside the inclusion are given by the following set (Jiang 2016, Eqs.13 there), called the exterior solutions to the Eshelby problem (see Fig. 3.1):

\[
\begin{align*}
\tilde{\varepsilon}(x) &= S^E(x) : S^{-1} : \varepsilon \\
\tilde{w}(x) &= \Pi^E(x) : S^{-1} : \varepsilon \\
\tilde{p}(x) &= \Lambda^E(x) : C : S^{-1} : \varepsilon
\end{align*}
\]

where the superscript E stands for exterior; because the exterior fields are not uniform \( S^E(x), \Pi^E(x), \) and \( \Lambda^E(x) \) all depend on location.

**Figure 3.1**: The Eshelby inclusion problem of an ellipsoidal RDE in a HEM and symbols used in partitioning Eqs.3.1 and 3.2. \( C_{ijkl}^{in} \) and \( C_{ijkl} \) are the viscous stiffness of the RDE and HEM respectively. The far-field mechanical state is defined by upper case symbols \( \Sigma, E, W, \) and \( P \), denoting respectively the deviatoric stress, strain rate, vorticity, and pressure. The constant mechanical fields inside the ellipsoid (the interior fields) are denoted by corresponding lower case symbols, \( \sigma, \varepsilon, w, \) and \( p \), and the difference fields are represented by \( \tilde{\sigma} = \sigma - \Sigma \), \( \tilde{w} = w - W \), and \( \tilde{p} = p - P \). The mechanical fields around the inclusion (exterior fields) vary with the position vector \( x \) and are expressed such as \( p(x) \) and \( \tilde{p}(x) = p(x) - P \).
The partitioning equations were derived for linearly viscous materials only. With a linearization approach (Jiang, 2016, 2014, 2013; Lebensohn and Tomé, 1993), Eqs. 3.1 and 3.2 can be extended to non-linear such as power-law viscous materials. In this case, a linearized viscosity such as the tangent viscosity (e.g., Jiang and Bentley, 2012) is used in the partitioning equations. Earth’s lithosphere is rheologically heterogeneous, in our application in this paper, it is understood that the macroscale medium surrounding an RDE is a hypothetical homogeneous-equivalent medium (HEM) (Lebensohn and Tomé, 1993; Molinari et al., 1987) whose rheology is obtained using a self-consistent homogenization from the rheologies of the constituent RDEs. The partitioning equations thus describe the interactions between the RDE with the hypothetical HEM. Numerical calculations using Eqs. 3.1 and Eqs. 3.2 are realized using MATLAB and Mathcad scripts, the algorithms for which are in the literature (Jiang, 2016, 2014, 2007; Jiang and Bentley, 2012; Qu et al., 2016). The calculations in this paper are based on these algorithms implemented in MATLAB. New MATLAB code for evaluation of pressure fields around the RDE embedded in a general anisotropic HEM has been developed in Chapter-2.

3.3 Limiting cases

Before we use the formal solutions of Eqs. 3.1 and 3.2 to investigate the pressure deviation in general situations, it is instructive to consider two limiting cases in 3D deformation. The first limiting case is an infinitely weak (inviscid) RDE in the HEM. As an inviscid RDE supports no deviatoric stress \( \tilde{\sigma} = 0 \), \( \tilde{\sigma} = -\Sigma \) (recall that \( \Sigma \) is the far-field stress tensor, Fig.3.1) and Eq. 3.1c becomes:

\[
\tilde{p}_{\text{inviscid}} = \Lambda \cdot C \cdot (J^d - S)^{-1} : C^{-1} : \Sigma \quad (3.3)
\]

The second limiting case is an infinitely strong (rigid) RDE in the HEM where \( \varepsilon = 0 \) hence \( \tilde{\varepsilon} = -\varepsilon \) (the far-field strain rate). In this case, Eq.3.1c yields

\[
\tilde{p}_{\text{rigid}} = -\Lambda \cdot C \cdot S^{-1} : \varepsilon \quad (3.4)
\]
Considering the case of an isotropic Newtonian HEM where $C = 2\eta J^d$ and $\Sigma = 2\eta E$ ($\eta$ being the HEM Newtonian viscosity), Eqs 3.3 and 3.4 lead to:

$$
p_{\text{invicid}}^{\text{iso}} = -\Psi : \Sigma \quad \text{(3.5a)}
$$

$$
p_{\text{rigid}}^{\text{iso}} = -\Lambda : \sigma \quad \text{(3.5b)}
$$

where $\Psi = \Lambda : (S - J^d)^{-1}$.

Both $\Psi$ and $\Lambda$ are related to the shape of the RDE only. $\Lambda$ is diagonal ($\Lambda_{ij} = 0$, if $i \neq j$) and satisfies $\Lambda_{11} + \Lambda_{22} + \Lambda_{33} = -1$ (Jiang, 2016). The components of $(S - J^d)^{-1}$ can be obtained from Jiang (2016, Eqs.33-34 there) which, together with the property of $\Lambda$, makes $\Psi$ always traceless ($\Psi_{11} + \Psi_{22} + \Psi_{33} = 0$) and diagonal ($\Psi_{ij} = 0$, if $i \neq j$).

Calculated components of $\Psi_{ij}$ and $\Lambda_{ij}$ in the RDE’s coordinate system are given in Table 3.1 for a few RDE shapes. It can also be seen that $|\Psi_{ii}| \leq 1$ (for $i = 1, 2, 3$). One can explicitly rewrite Eq. 3.5a as $p = -(\Psi_{11} \Sigma_{11} + \Psi_{22} \Sigma_{22} + \Psi_{33} \Sigma_{33})$. For a spherical RDE, $p = 0$ because all components of $\Psi$ are zero. In a general triaxial ellipsoid with three axes ($a_1 > a_2 > a_3$), $\Psi_{11} < \Psi_{22} < \Psi_{33}$. For a spheroid RDE, the distinct $\Psi_{ij}$ components are $-\Psi_{11} = 2\Psi_{22} = 2\Psi_{33} > 0$ for a prolate ($a_1 > a_2 = a_3$) and $\Psi_{11} = \Psi_{22} = -\frac{1}{2} \Psi_{33} < 0$ for an oblate ($a_1 = a_2 > a_3$) case. The extremum values of $\tilde{p}$ occur when the RDE principal axes are aligned with the principal directions of $\Sigma$ and

$$
\tilde{p}_{\text{extremum}} = - (\Psi_{11} \Sigma_i + \Psi_{22} \Sigma_j + \Psi_{33} \Sigma_k)
$$

where $\Sigma_i$, $\Sigma_j$, and $\Sigma_k$ are three principal deviatoric stresses. For an infinitely flat oblate ellipsoid (a layer), $\Psi_{11} = \Psi_{22} = -\frac{1}{3}$ and $\Psi_{33} = \frac{2}{3}$ (Table 3.1) which yields $-\Sigma_i \leq \tilde{p} = -\Sigma_3$.

For a rod-like prolate RDE, $\Psi_{11} = -\frac{1}{3}$ and $\Psi_{22} = \Psi_{33} = \frac{1}{6}$ (Table 3.1) which yields
0.5\Sigma_3 \leq \tilde{p} \leq 0.5\Sigma_1. As a general triaxial ellipsoid lies between an infinitely flat oblate ellipsoid and a rod-like prolate body, one can conclude that in a general extremely weak (inviscid) triaxial element, the pressure deviation can be expressed as \( \min \{ -\Sigma_i, 0.5\Sigma_3 \} \leq \tilde{p} \leq \max \{ -\Sigma_i, 0.5\Sigma_1 \} \). The lower limit \( \min \{ -\Sigma_i, 0.5\Sigma_3 \} \) is the highest under-pressure and the upper limit \( \max \{ -\Sigma_i, 0.5\Sigma_1 \} \) is the highest overpressure the RDE can have. Note that tensile stress is positive in this paper, following the convention of continuum mechanics (\( \Sigma_1 \), \( \Sigma_2 \), and \( \Sigma_3 \) are the deviatoric maximum principal tensile stress, deviatoric intermediate principal stress, and the deviatoric maximum compressive stress respectively).

Similar analysis can be made for endmember rigid inclusions. Because of the properties of \( \Lambda \), Eq. 3.5b can be explicitly written as \( \tilde{p} = -\left( \Lambda_{i1}\sigma_{i1} + \Lambda_{i2}\sigma_{i2} + \Lambda_{i3}\sigma_{i3} \right) \). It is also clear that \(-1 \leq \Lambda_{ii} \leq 0\) (for \( i = 1, 2, 3 \)) always holds (Table 3.1). Thus, for a spherical RDE, \( \tilde{p} = 0 \) as \( \Lambda_{i1} = \Lambda_{i2} = \Lambda_{i3} = -\frac{1}{3} \). In an ellipsoid, a larger \( |\Lambda_{ii}| \) (i.e., closer to 1) corresponds to a shorter ellipsoid principal axis. The extremum values of \( \tilde{p} \) occur when the RDE’s principal axes are aligned with the principal deviatoric stresses \( \sigma_1 \), \( \sigma_2 \), and \( \sigma_3 \) in the RDE. For a layer-like RDE, \( \Lambda_{i1} = \Lambda_{i2} = 0 \) and \( \Lambda_{i3} = -1 \) yielding \( \sigma_3 \leq \tilde{p} \leq \sigma_1 \), and for a rod-like RDE, \( \Lambda_{i1} = 0 \) and \( \Lambda_{i2} = \Lambda_{i3} = -0.5 \) giving \( -0.5\sigma_1 \leq \tilde{p} \leq -0.5\sigma_3 \). For a general triaxial RDE, the pressure deviation can be expressed as: \( \min \{ -0.5\sigma_1, \sigma_3 \} \leq \tilde{p} \leq \max \{ \sigma_1, -0.5\sigma_3 \} \).

Rheologically, a real RDE always lies between the inviscid and rigid cases. The above analysis is therefore a formal proof that in a Newtonian matrix, the pressure deviation in an ellipsoid inclusion is always equal or below the principal deviatoric stresses in the matrix or in the inclusion itself. The analysis does not consider the pressure deviation outside the RDE nor in an anisotropic and non-Newtonian matrix. These general cases are considered numerically below, using Eqs. 3.1 and 3.2.
### Table 3.1: Components of $\psi_{ij}$ and $\Lambda_{ij}$ for various RDE shapes.

<table>
<thead>
<tr>
<th>Shape</th>
<th>Axial Ratios</th>
<th>$\psi$</th>
<th>$\Lambda$</th>
</tr>
</thead>
</table>
| **Prolate Ellipsoid**  | 3:1:1        | \[
\begin{pmatrix}
-0.281 & 0 & 0 \\
0 & 0.140 & 0 \\
0 & 0 & 0.140
\end{pmatrix}
\] | \[
\begin{pmatrix}
-0.109 & 0 & 0 \\
0 & -0.446 & 0 \\
0 & 0 & -0.446
\end{pmatrix}
\] |
|                        | 10:1:1       | \[
\begin{pmatrix}
-0.328 & 0 & 0 \\
0 & 0.164 & 0 \\
0 & 0 & 0.164
\end{pmatrix}
\] | \[
\begin{pmatrix}
-0.02 & 0 & 0 \\
0 & -0.49 & 0 \\
0 & 0 & -0.49
\end{pmatrix}
\] |
|                        | $\infty$:1:1 | \[
\begin{pmatrix}
-0.333 & 0 & 0 \\
0 & 0.167 & 0 \\
0 & 0 & 0.167
\end{pmatrix}
\] | \[
\begin{pmatrix}
0 & 0 & 0 \\
0 & -0.5 & 0 \\
0 & 0 & -0.5
\end{pmatrix}
\] |
| **Oblate Ellipsoid**   | 3:3:1        | \[
\begin{pmatrix}
-0.242 & 0 & 0 \\
0 & -0.242 & 0 \\
0 & 0 & 0.484
\end{pmatrix}
\] | \[
\begin{pmatrix}
-0.182 & 0 & 0 \\
0 & -0.182 & 0 \\
0 & 0 & -0.635
\end{pmatrix}
\] |
|                        | 10:10:1      | \[
\begin{pmatrix}
-0.324 & 0 & 0 \\
0 & -0.324 & 0 \\
0 & 0 & 0.648
\end{pmatrix}
\] | \[
\begin{pmatrix}
-0.07 & 0 & 0 \\
0 & -0.07 & 0 \\
0 & 0 & -0.86
\end{pmatrix}
\] |
|                        | $\infty$:1:1 | \[
\begin{pmatrix}
-0.333 & 0 & 0 \\
0 & -0.333 & 0 \\
0 & 0 & 0.666
\end{pmatrix}
\] | \[
\begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & -1
\end{pmatrix}
\] |
| **Triaxial Ellipsoid** | 5:3:1        | \[
\begin{pmatrix}
-0.299 & 0 & 0 \\
0 & -0.237 & 0 \\
0 & 0 & 0.535
\end{pmatrix}
\] | \[
\begin{pmatrix}
-0.104 & 0 & 0 \\
0 & -0.209 & 0 \\
0 & 0 & -0.687
\end{pmatrix}
\] |
|                        | 10:3:1       | \[
\begin{pmatrix}
-0.324 & 0 & 0 \\
0 & -0.234 & 0 \\
0 & 0 & 0.559
\end{pmatrix}
\] | \[
\begin{pmatrix}
-0.042 & 0 & 0 \\
0 & -0.232 & 0 \\
0 & 0 & -0.726
\end{pmatrix}
\] |
|                        | 500:100:1    | \[
\begin{pmatrix}
-0.333 & 0 & 0 \\
0 & -0.333 & 0 \\
0 & 0 & 0.667
\end{pmatrix}
\] | \[
\begin{pmatrix}
0 & 0 & 0 \\
0 & -0.01 & 0 \\
0 & 0 & -0.99
\end{pmatrix}
\] |

3.4 Pressure deviations in and outside rheologically heterogeneous elements

As it is clear from Eqs. 3.1c and 3.2c that the pressure deviation is unaffected by the vorticity of the imposed flow, it is sufficient to consider macroscale pure-shearing flows only. The macroscale pure shearing flow is defined in a coordinate system XYZ (Fig. 3.2). Because we are most concerned with the extremum pressure deviations inside and around an RDE and, for isotropic HEMs, the extremum pressures are attained when at
least one of RDE’s semi-axes is parallel to one principal strain rate axis of the imposed flow, we let the $a_1$ axis parallel to the coordinate Z-axis (Fig. 3.2) without any loss of generality. In our numerical investigations on anisotropic HEMs below, we will ensure that one symmetric axis of the HEM’s anisotropy is parallel to the coordinate Z-axis so that letting the RDE’s $a_1$ axis parallel to the coordinate Z leads to no loss of generality either. Thus, in all our numerical investigations, the orientation of the RDE is defined by angle $\theta$ between $a_2$ axis and the X coordinate axis (Fig. 3.2). We investigate the pressure deviations inside and around the RDE as $\theta$ and HEM rheology vary. The second invariant of the deviatoric stress in the HEM, $\Sigma_{II} = \sqrt{\frac{1}{2} \Sigma_{ij} \Sigma_{ij}}$, or in the RDE, $\sigma_{II} = \sqrt{\frac{1}{2} \sigma_{ij} \sigma_{ij}}$, is used to normalize the pressure deviation fields in the following.

Figure 3.2: Geometry of the plane-strain pure shearing flow and the RDE considered in the numerical investigation. The flow is in the XY plane with principal strain rate axes parallel to the X- and Y-axis. The RDE’s $a_1$-axis is parallel to Z and $\theta$ is the angle between $a_2$ and the X-axis. All flow fields referred to in the paper are defined in the XYZ system.
3.4.1 Pressure deviation in a Newtonian HEM and verification of the numerical approach

Previous work on pressure fields inside and around an inclusion was limited to 2D ellipses in a Newtonian isotropic matrix (Schmid and Podladchikov, 2003; Mancktelow 2008) or a Newtonian matrix of planar anisotropy (Fletcher 2009; Jiang 2016). We first apply our general numerical approach to the pressure fields in an ellipsoid in the Newtonian matrix and use previous 2D results as means of verification of the approach in this paper. In such case, the rheological contrast of the RDE to the HEM is given by a viscosity ratio \( r \). Fig. 3.3 shows the XY-cross sections of the pressure deviations related, respectively, to a weaker (\( r = 0.01 \), left column, Figs. 3.3a-d) and stronger (\( r = 100 \), Figs. 3.3e-h) RDE as \( \theta \) varies from 0° to 90° with an increment of 30° counter-clockwise. The axial ratios of the RDE are 10:5:1 (aspect ratio of 5:1 in the XY section). The pressure deviation \( \frac{\tilde{p}}{\Sigma_{II}} \) is always below 1 inside the weak RDE and below 2.5 outside it. Numerical calculations for very large aspect ratios (>100:1, not shown here) show that the exterior \( \frac{\tilde{p}}{\Sigma_{II}} \) is below 7 around weak RDEs when the RDE is in the direction of maximum shear stress. For the strong RDE, the maximum interior \( \frac{\tilde{p}}{\sigma_{II}} \) can reach high values as the aspect ratio of the RDE increases but \( \frac{\tilde{p}}{\sigma_{II}} \) is always below 1 (see Fig 3.4 below). The exterior \( \frac{\tilde{p}}{\Sigma_{II}} \) around the strong RDE is below 4 and \( \frac{\tilde{p}}{\sigma_{II}} \) is below 1.5. Additional numerical calculations (not presented) show that \( \frac{\tilde{p}}{\sigma_{II}} \) is below 1.2 even for extremely high aspect ratios (>100:1). These results are in excellent agreement with previous work based on 2D and Newtonian rheology (e.g., Schmid and Podladchikov, 2003; Mancktelow 2008).
Figure 3.3: The XY-section of pressure deviation fields \( \left( \frac{\tilde{p}}{\Sigma_{\|}} \right) \) related to a RDE in an isotropic HEM under pure shearing flow. The RDE’s axial ratios are 10:5:1 (sectional aspect ratio 5:1 in the XY plane) (a)-(d) The sectional pressure fields \( \left( \frac{\tilde{p}}{\Sigma_{\|}} \right) \) where the RDE is weak \((r=0.01)\) as \( \theta \) changes from \( \theta = 0^\circ \) to \( \theta = 90^\circ \) with interval of 30° counter-clockwise. (e)-(h): Same plots as (a)-(d) where the RDE is strong \((r = 100)\).
3.4.2 Pressure deviation in a power-law isotropic HEM

It turns out that the pressure deviation fields in and outside an RDE (Newtonian or power-law) embedded in an isotropic power-law HEM are similar in pattern to those presented in Fig. 3.3 for isotropic Newtonian HEMs but with an overall reduction in the strength of pressure. This can be understood by comparing Eq. 3.1c (or 3.2c) between Newtonian and power-law HEM cases. For isotropic HEMs, Eq. 3.1c becomes:

\[
\bar{p}_{\text{powerlaw}} = \frac{2\eta}{n} \Lambda : S^{-1} : \bar{\varepsilon}_{\text{powerlaw}} 
\]

(3.6a)

\[
\bar{p}_{\text{Newtonian}} = 2\eta \Lambda : S^{-1} : \bar{\varepsilon}_{\text{Newtonian}}
\]

(3.6b)

where \( \eta \) is the Newtonian or effective viscosity of the HEM. The \( \Lambda : S^{-1} \) term is identical whether the HEM is Newtonian or power-law. \( \bar{\varepsilon}_{\text{powerlaw}} \) certainly differs from \( \bar{\varepsilon}_{\text{Newtonian}} \) if the RDE itself is power-law viscous as the effective viscosity ratio is no longer constant. But this does not change the pattern of the pressure distribution. The biggest effect of a power-law HEM is that the tangent viscosity, \( \frac{\eta}{n} \), rather than the secant (or effective) viscosity of the HEM applies to the interaction equations, which leads to an overall reduction in the strength of the pressure field in and around an RDE. Fig. 3.4a shows how \( \bar{p} \) inside the RDE is affected by effective viscosity ratio \( r_{eff} \) for a Newtonian \((n=1)\) HEM and Fig. 3.4b for a power-law HEM \((n=3)\). The effect of viscosity ratio on the interior \( \bar{p} \) is only significant in the range of \( 0.01 < r_{eff} < 100 \). Increasing \( r_{eff} \) over 100 or decreasing it below 0.01 has little effect on the interior field of pressure deviation. \( \bar{p} / \Sigma_{\mu} \) for a weak RDE and \( \bar{p} / \sigma_{\mu} \) for a strong RDE are always below unity. Fig. 3.4c plots the maximum \( \bar{p} \) as a function of the HEM’s power-law stress exponent for different shaped RDEs. \( \bar{p} / \Sigma_{\mu} \) is insensitive to \( n \) for weak RDEs whereas \( \bar{p} / \sigma_{\mu} \) decreases with increasing \( n \) for strong RDEs.
A rheologically anisotropic material can vary in symmetry from the lowest triclinic to being fully isotropic (Mura, 1987, p. 129-176; Ting, 1996). Little is known about the anisotropic viscosity of rocks. To gain an understanding of how the results obtained above, based on isotropic HEMs, may be affected by rheological anisotropy, we consider two cases of HEM anisotropy. Our purpose is to find out whether HEM anisotropy will increase or decrease the pressure deviation relative to the isotropic HEM.

3.4.3 Pressure deviation in a power-law anisotropic HEM

Figure 3.4: Pressure field inside RDEs, of various shapes, as a function of (a) effective viscosity ratio ($r_{\text{eff}}$) for a Newtonian HEM ($n=1$), (b) effective viscosity ratio ($r_{\text{eff}}$) for a power-law HEM with $n=3$, and (c) the HEM power-law stress exponent ($n$). $\tilde{p}/\sigma_{II}$ or $\tilde{p}/\Sigma_{II}$ is always below 1. See text for more details.

A rheologically anisotropic material can vary in symmetry from the lowest triclinic to being fully isotropic (Mura, 1987, p. 129-176; Ting, 1996). Little is known about the anisotropic viscosity of rocks. To gain an understanding of how the results obtained above, based on isotropic HEMs, may be affected by rheological anisotropy, we consider two cases of HEM anisotropy. Our purpose is to find out whether HEM anisotropy will increase or decrease the pressure deviation relative to the isotropic HEM.
The first is a simple yet geologically common case of anisotropy expected in well-layered or foliated rocks (Fig.3.5a, e.g., Johnson and Fletcher, 1994) with two distinct viscosities: a normal viscosity $\eta_N$ and a shear viscosity $\eta_s$. The former measures the material’s resistance to layering parallel shortening or extension and the latter measures the resistance to layering parallel shear. $m = \eta_s / \eta_N$ measures the strength of the anisotropy. For rocks, it is reasonable to assume that $m \geq 1$ as shortening or extension parallel to the layering is thought to be stronger than simple shearing along it. We consider the case where the RDE itself is isotropic with an effective viscosity $\eta_{\text{eff}}$ below.

Fig.3.5 shows pressure fields calculated for an elliptical cylinder in the above-mentioned planar anisotropic HEM undergoing pure shearing flow (Fig. 3.5a). For comparison, Figs.3.5b and c are pressure fields related to $r_{\text{eff}} = 0.1$ and $r_{\text{eff}} = 10$ in the isotropic HEM ($m=1$). Figs.3.5d-g are pressure fields $\tilde{p} / \Sigma_{II}$ for the weak RDE ($r_{\text{eff}} = 0.1$) in the HEM with $m=10$ as $\theta$ varies from 0° (Fig.3.5d) to 90° (Fig.3.5g) with an increment of 30° counter clockwise. Figs.3.5h-k are corresponding pressure fields $\tilde{p} / \Sigma_{II}$ for the strong RDE ($r_{\text{eff}} = 10$) in the same anisotropic HEM as $\theta$ varies. Full 3D pressure fields for a weak ($r_{\text{eff}} = 0.1$) RDE with axial ratios 6:3:2 are shown in Fig.3.6. Figs.3.6a-c shows the 3D pressure iso-surfaces and cross-sections for the RDE in an isotropic ($m=1$) HEM. Figs.3.6d-f are similar plots as Figs.3.6a-c but for a planar anisotropic ($m=10$) HEM. It can be seen clearly from Figs.3.5 and 3.6 that the pressure fields in the anisotropic HEM situation are universally weaker than the isotropic HEM situation. As the anisotropy strength $m$ increases, the pressure deviation fields decrease for all viscosity ratios between the RDE and the HEM (Fig.3.7).
Figure 3.5: The pressure deviation fields related to weak and strong elliptical cylinders in a planar anisotropic HEM under pure shearing flow. (a) The geometric relation between the flow field, RDE, and anisotropy. The anisotropy plane is perpendicular to the paper and horizontal. The principal strain rates of the pure shearing flow are parallel (horizontal) and perpendicular (vertical) to the anisotropy plane. The cylindrical axis of RDE lies in the anisotropy and the sectional ellipse’s long axis is at θ relative to the anisotropy. (b) and (c): Pressure fields related to a weak ($r_{\text{eff}} = 0.1$) and strong RDE ($r_{\text{eff}} = 10$) both at θ=0°, respectively, in a HEM with $m = 1$ (isotropic) for comparison. (d)-(g): Pressure fields related to the weak RDE in a HEM with $m=10$, as θ changes from 0° to 90° counterclockwise with interval of 30°. (h)-(k): Same plots as (d)-(g) but for a strong RDE. The sectional ratio of the RDE is 5:1 for all plots.
Figure 3.6: 3D pressure fields related to a weak RDE (effective viscosity ratio $r_{\text{eff}} = 0.1$) with axial lengths 6:3:2) in an isotropic ($m=1$) HEM (left column) and in a planar anisotropic ($m=10$) HEM (right column) under pure shearing flow. The HEM anisotropy plane is parallel to the XZ plane of Fig.3.2. (a): Plot of 3D iso-pressure surfaces $\tilde{p}/\Sigma_n = -0.4, 0, 0.4$ (in purple, green, and yellow, respectively) for the isotropic HEM case. The gray surface is the weak RDE. The $\tilde{p}/\Sigma_n = 0$ surface separates the positive pressure deviation from the negative pressure deviation domains. (b) and (c) continued in next page.
The second case of anisotropic HEM is one generated by a self-consistent homogenization procedure (Jiang, 2014). We consider a macroscale representative volume of HEM composed of 200 RDEs. The initial shapes of these RDEs are with $a_1 = 10$, $a_2 = 1$ and $a_3$ varying randomly from 1 to 10. The initial orientations are random in 3D space. The relative viscosities, at the given bulk strain rate, vary uniformly between 1 and 10 and the power-law stress exponents vary uniformly between 1 and 4. Such a range of relative viscosities together with the stress exponent variation will yield a maximum effective viscosity range of $10^4$. This initial assemblage of RDEs is submitted to a simple shearing deformation (with shear plane parallel to the XZ plane and shear direction along X positive, Fig. 3.2) to reach a shear strain of 10. At this strain, the RDEs

(b) and (c): Respectively, the XY and XZ cross sections of the pressure fields for the isotropic HEM case. (d)-(f): Corresponding plots to (a)-(c) for the planar anisotropic HEM case ($m=10$). Compared to the isotropic HEM situation, the pressure fields related to the RDE in the anisotropic HEM situation are universally reduced. Note the (a)-(c) set of plots and the (d)-(f) set of plots use independent scale bars for pressure strength.

Figure 3.7: (a) The pressure fields inside a cylindrical RDE in a planar anisotropic HEM (geometry shown in Fig.5a) as a function of $\theta$, for a weak ($r_{\text{eff}} = 0.1$, dashed lines) and strong ($r_{\text{eff}} = 10$, solid lines) RDE respectively, for various $m$. As $m$ increases, the pressure field strength decreases. (b) The RDE interior pressure decreases with increasing HEM’s $m$, irrespective of the relative viscosity ratios.

The second case of anisotropic HEM is one generated by a self-consistent homogenization procedure (Jiang, 2014). We consider a macroscale representative volume of HEM composed of 200 RDEs. The initial shapes of these RDEs are with $a_1 = 10$, $a_2 = 1$ and $a_3$ varying randomly from 1 to 10. The initial orientations are random in 3D space. The relative viscosities, at the given bulk strain rate, vary uniformly between 1 and 10 and the power-law stress exponents vary uniformly between 1 and 4. Such a range of relative viscosities together with the stress exponent variation will yield a maximum effective viscosity range of $10^4$. This initial assemblage of RDEs is submitted to a simple shearing deformation (with shear plane parallel to the XZ plane and shear direction along X positive, Fig. 3.2) to reach a shear strain of 10. At this strain, the RDEs
are aligned with a shape-preferred orientation about 6° counterclockwise from the X-axis. Although all the constituent elements of the HEM are isotropic, because of finite strain and preferred shape fabric buildup, the HEM is statistically monoclinic. The homogenized viscosity of the HEM, $C_m$, using the approach described in Jiang (2014, 2016) is a fourth-order tensor. The viscosity contrast between the RDE and such HEM is a tensor quantity. We define an invariant viscosity for the HEM using the stress and strain rate invariants as $\eta = \frac{\Sigma \mu}{2E_{il}}$. The viscosity ratio of an isotropic RDE to the HEM can then be expressed as $r_{eff} = \frac{\eta_{RDE}}{\eta}$. Fig. 3.8a shows the XY section of the pressure deviation field related to an isotropic RDE (6:3:2) isotropic (the aspect ratio in the XY plane is 3:2), with $r_{eff} = 0.1$. The bulk flow is pure shearing as in Fig. 3.2 and the RDE is at $\theta = 0°$. The exterior pressure field has a monoclinic symmetry consistent with the fact that $C_m$ was generated by simple shearing and the pressure pattern is aligned with the shape-preferred orientation of the HEM which is about 6° counterclockwise relative to the horizontal (the dashed white line in Fig.3.8a). Fig.3.8b shows the pressure deviation fields inside RDEs, all with the same shape (6:3:2) but with varying relative viscosities. Solid and dashed lines are for the anisotropic and isotropic HEMs respectively. The internal pressure fields are universally reduced in the anisotropic HEM cases. Comparing Fig.3.8a against the corresponding isotropic case (Fig.3.6b), the strength of the exterior pressure deviation field is also subdued in the anisotropic situation.
Note that as we are concerned with the maximum values of pressure deviations in this work, Figs. 3.3-3.8 present the instantaneous pressure deviation fields. In a natural setting, the RDE will deform depending on its rheological contrast with the HEM, shape, and orientation with respect to the far-field flow in the HEM, and pressure deviations in and around the RDE may vary with time. Our approach can be readily used to simulate such pressure deviations if required for a specific problem.

Figure 3.8: (a): The XY-plane cross section of the $\tilde{p}/\Sigma_\parallel$ field related to a RDE with axial ratios of 6:3:2. The RDE is oriented at $\theta=0^\circ$ and undergoes pure shear flow as in Fig. 3.2. The RDE is itself isotropic with a relative viscosity 0.1 times the invariant viscosity of the HEM as defined in the text. The rheological property of the HEM is generated by the MOPLA self-consistent procedure (see text for more description). The dashed white line indicates the preferred shape fabric of the HEM. The pattern of the pressure field is monoclinic and in the orientation of the HEM anisotropy. (b): The pressure deviation $\tilde{p}/\Sigma_\parallel$ fields inside RDEs, all with the same shape (6:3:2) but with varying relative viscosities (viscosity ratios, $r_{eff}$ all with respect to the invariant viscosity of the HEM). Solid and dashed lines are for the anisotropic and isotropic HEMs respectively. The pressure fields are uniformly subdued in the anisotropic HEM, compared to their isotropic HEM situations.
3.5 Discussion

We have shown analytically that in a Newtonian matrix, the pressure deviation in an ellipsoid inclusion is always equal to or below the principal deviatoric stresses in the matrix or in the inclusion itself. In general power-law and anisotropic HEMs, we have demonstrated that the pressure deviation in any given RDE is always limited by and of a similar order to the local ($\sigma_{II}$) or ambient ($\Sigma_{II}$) deviatoric stress invariant. The pressure deviation inside a weak RDE is always less than the deviatoric stress invariant of the ambient medium ($\tilde{p}/\Sigma_{II} < 1$) regardless of the element’s shape, orientation, and power-law stress exponent. Around a weak RDE, $\tilde{p}/\Sigma_{II}$ is usually below 3 and never above 7 even for extremely flat or elongate RDEs. The maximum exterior pressure affects a very small volume near the tips of a flat or elongated RDE. For strong RDEs, the pressure deviation inside them is always less than the element’s deviatoric stress invariant ($\tilde{p}/\sigma_{II} < 1$) regardless of the RDE’s shape and orientation. The pressure deviation outside a strong RDE is always below 1.5. The pressure deviation in a strong RDE decreases rapidly as the power-law stress exponent of the HEM increases. The magnitude of pressure deviation in materials with planar or monoclinic anisotropy is smaller than the pressure deviation in isotropic materials. Therefore, we can generally state that the maximum pressure deviations, as a result of bulk deviatoric stress (i.e., arising from imposed bulk deformation), are on the same level as the deviatoric stress in the deforming system.

The discovery that $\tilde{p}/\Sigma_{II} \leq 1$ inside a weak RDE regardless of its shape, viscosity ratio, orientation, and the power-law stress exponent of the surrounding HEM has implications for the tectonic pressures in narrow deforming zones of weak materials. Previous investigations on transpressional zones and subduction channels have applied the analytical solution of Jaeger (1969, p. 140-149) for a Newtonian fluid between rigid parallel walls approaching one another. This model leads to extremely high-pressure deviations (Robin and Cruden, 1994; Mancktelow, 2008, 1995, 1993) even if the wall rock deformation is considered (Raimbourg and Kimura, 2008). If such narrow zones are viewed approximately as extremely flat RDEs of low viscosity material embedded in a...
stronger lithospheric HEM, our results would suggest that the pressure deviations in these zones are always below the deviatoric stress invariant in the country-rock. The significant difference between the micromechanical approach based on the Eshelby formalism that we have taken in this paper and the application of Jaeger’s (1969) solution is that in the former the interactions between the deforming zone and the country-rock HEM are addressed by the partitioning equations whereas in the latter the interactions depend on the assigned boundary conditions.

Both $\sigma_{II}$ and $\Sigma_{II}$ are limited by the strength of rocks. Unfortunately, there are still great controversies on their level in Earth’s lithosphere, especially over the long-term (Ma) time scale. Differential stress (which is equal to two times of the deviatoric stress invariant used in this paper if a plane-straining deformation is assumed) estimates based on a variety of techniques and measurements have yielded results from ~10 MPa to 150 MPa (e.g., Behr and Platt, 2014; Hasegawa et al., 2011; Lamb, 2006; Seno, 2009). If they are used as the HEM and RDE stress range, they would correspond to a minor $\tilde{p}$ in nature according to our work. On the other hand, if GPa-level deviatoric stresses are assumed (e.g., Andersen et al., 2008; Moghadam et al., 2010), our work would predict correspondingly GPa-level pressure deviations on the RDE scale. However, there is evidence suggesting that these high differential stresses are due to transient strong interactions and do not represent the long-term tectonic stress. The differential stress estimate of Andersen et al. (2008) is based on energy release measurement from fault-offsets during pseudotachylyte formation, clearly reflecting a transient event. Moghadam et al. (2010) obtained GPa-level differential stresses from the extrapolated flow law of experimentally deformed omphacite aggregates. They have pointed out explicitly that based on geological observations (Stöckhert, 2002), the high stresses are likely due to subduction seismicity.

The mechanical interaction between an RDE and the HEM is fundamentally different from the scenario of high-pressure and ultrahigh-pressure (UHP) mineral phases enclosed in a rigid mineral like diamond and zircon (Parkinson and Katayama 1999; Zhukov and Korsakov 2015). The rigid mineral serves as a pressure vessel to preserve the enclosed high-pressure assemblages (Zhang, 1998) while the strength of the poly-grain HEM
embedding the vessel is irrelevant. That is, there is negligible interaction between the HEM and the phases inside the pressure vessel. The situation of a weak RDE in contact with or surrounded by some strong mineral grains in the HEM is entirely different. In this case, the interaction is still one between the RDE and the HEM although the neighboring strong grains may induce high-order interactions above the RDE-HEM approximation. In micromechanics, the high-order interactions are considered secondary (Lebensohn and Tomé, 1993; Mura, 1987; Nemat-Nasser and Hori, 1999). The laboratory setup of a weak sample clamped between strong anvils (e.g., Ji and Wang, 2011) mimics the pressure vessel effect and cannot be used as an analog to the situation of a quartz grain in contact with neighboring garnet grains in natural metamorphic rocks.

The pressure deviation \( \ddot{p} \) in this paper is the difference of pressure in or around an RDE from the ambient macroscale pressure. Strictly, \( \ddot{p} \) is not the so-called tectonic over- or under-pressure unless the ambient macroscale pressure is lithostatic. However, only \( \ddot{p} \) is directly relevant to petrological observations if it is greater than the geobarometric resolution. The absolute over- or under-pressure values, on the other hand, cannot be resolved from petrological records. Schmalholz et al. (2014b) apply force balance equations to consider tectonic-scale pressure deviations from the lithostatic pressure. Their analysis is based on plane-strain deformation and they obtained tectonic-scale pressure deviation of around 60-70 MPa. Denoting this pressure deviation by \( \ddot{p}_T \) and the lithostatic pressure \( P_L \), the HEM pressure can then be expressed as \( P = P_L + \ddot{p}_T \). The pressure deviation of this paper, \( \ddot{p} \), is the deviation of pressure from the ambient reference \( P \).

Because our investigation in this contribution is based on viscous rheology, the results apply only to geological processes with characteristic time scales much longer than the viscous relaxation time. If we regard the HEM effective viscosity as being between \( 10^{18} \) - \( 10^{22} \) Pas, assuming that its stress exponent is 3 and shear modulus 10GPa, the viscous relaxation time is between 1 and 10,570 years. Note one must use a linearized (such as tangent, see Jiang and Bentley, 2012) viscosity of the material to calculate its viscous relaxation time as the relaxation time concept is based on the linear theory of Maxwell.
viscoelasticity. Therefore, our conclusions should be valid for petrological processes on the Ma time scale. Viscoelastic interactions can be considered in a similar way as in this paper by using the approximate solutions of Molinari et al. (1997). The conclusion that \( \tilde{p} \) is on the same level as the deviatoric stress will remain true although elastic interactions will generate transient higher deviatoric stresses and correspondingly transient higher \( \tilde{p} \) which then decay following the transient interaction.

The assumptions of ellipsoids for RDEs and the use of HEM for the macroscale material may introduce some uncertainties in the actual \( \tilde{p} \). Our results represent averaged \( \tilde{p} \) in the RDE. Where the RDE is convex-shaped, the actual pressure variation in the element is small relative to the averaged field and our results can be regarded as good approximations to the actual pressure fields. Where an RDE is more irregularly shaped, more significant heterogeneous variations in \( \tilde{p} \) from the calculated average are possible. Since such pressure variations are always associated with deviatoric stress variations, they will be relaxed and homogenized rapidly. This is achieved by dynamical recrystallizations, neocrystallization, or the formation of other subgrain structures in minerals. At time scales much greater than the viscous relaxation, such pressure variations within and around an RDE are justifiably neglected. The use of HEM in our investigation means that we have ignored high-order local interactions – we have used a mean-field theory rather than one such as the N-site theory that accounts for high-order local interactions. More complicated formulation and much more computation resources are needed to consider such high-order theories. However, texture modeling of polycrystals has shown that considering high-order interactions does not lead to significant changes in the modeled texture. We regard this as evidence that the mean-field approach captures the first-order significant physics of the problem.

### 3.6 Pressure variation due to an initial pressure anomaly

The above investigation and discussion are related to the old problem of tectonic overpressure, namely pressure deviations caused by tectonic deformation, or equivalently, in a macroscale deviatoric stress field. More recently, there have been quite a few works on pressure deviations in the lithosphere caused by an initial pressure anomaly.
perturbation in a static stress state. The origin of the initial pressure perturbations has been ascribed to residual pressures in grains from rapid exhumation, a local volume-increasing metamorphic reaction, heterogeneous thermal expansion, and melting (e.g., Dabrowski et al., 2015). It is argued that the initial local pressure anomaly and a sharp pressure gradient may be preserved for a long time if the surrounding material has a large viscous relaxation time (Dabrowski et al., 2015; Tajčmanová et al., 2014). Claims have been made that such great grain-scale pressure fluctuations may even explain UHP metamorphism at normal crustal depth (e.g., Dabrowski et al., 2015; Tajčmanová et al., 2015, 2014). However, the large bulk modulus of minerals and rocks implies that initial extra_pressures in them, if generated, are largely released by infinitesimal elastic volume strains, without causing viscous flow in the surrounding material. Let us consider the kyanite crystals with an initial high-pressure deviation (Tajčmanová et al., 2014) as an example. Because kyanite has a large bulk modulus of ~200GPa (Liu et al., 2009), to release ~800MPa extra pressure (Tajčmanová et al., 2014) requires ~0.4% volume expansion, equivalent to barely 0.13% increase in grain size. Such an infinitesimal strain is readily accommodated by the surrounding polycrystal aggregates.

To analyze it more rigorously, the case of a strong and highly-pressured phase surrounded by a polyphase HEM, like the kyanite in quartz feldspar matrix of Tajčmanová et al. (2014), belongs to the problem of an inhomogeneity with eigenstrain which is treated in micromechanics texts and papers (e.g., Ma and Korsunsky, 2014; Mura, 1987). The initial pressure-induced volume strain in kyanite constitutes the eigenstrain and the kyanite grain is an inhomogeneity in Eshelby’s (1957, 1959) sense. Mura (1987, p. 179-184) gives the solutions for this type of problem in isotropic elastic materials. Ma and Korsunsky (2014) give an explicit relation for a spherical elastic inhomogeneity with radial eigenstrain (equivalent to an initial pressure anomaly) embedded in an isotropic elastic medium. The following equation is a recast of their Eq.3.12:

\[ \tilde{p}_r = \frac{4\mu}{4\mu + 3K^*} \tilde{p}_0 \]
where \( \tilde{p}_0 \) is the initial pressure deviation in the spherical inhomogeneity, \( \tilde{p}_r \) the equilibrated residue pressure deviation, \( \mu \) the elastic shear modulus of the matrix, and \( K^* \) is the bulk modulus of the inhomogeneity. Taking \( \mu = 10 \text{GPa}, K^* = 200 \text{GPa} \) for the situation of kyanite in a HEM of quartz feldspar aggregate, one gets \( \tilde{p}_r \approx 0.06 \tilde{p}_0 \). This means that the initial pressure perturbation, say, \( \tilde{p}_0 = 800 \text{MPa} \), is reduced to a residue pressure of \( \tilde{p}_r \approx 48 \text{MPa} \) by an instantaneous elastic interaction with the matrix. Note the response of a viscoelastic body to a sudden disturbance such as a discontinuous pressure anomaly is primarily elastic (e.g., Molinari et al., 1997). Therefore, if one considers the persistence of the pressure deviation in kyanite due to the viscous relaxation of the surrounding rocks (Dabrowski et al. 2015), then it is \( \tilde{p}_r \), not \( \tilde{p}_0 \), that is relevant. The residual pressure deviation (\( \tilde{p}_r \approx 48 \text{MPa} \)) is too low to cause the chemical zoning of plagioclase as claimed by Tajčmanová et al. (2014).

The \( \frac{4\mu}{4\mu+3K^*} \) term is always below 1. All natural rocks and minerals have large bulk moduli and in the case of a strong phase in a weak HEM, \( \tilde{p}_r \ll \tilde{p}_0 \). One can generally expect that most of \( \tilde{p}_0 \) are relaxed elastically. In the event the local pressure perturbation is in a phase with lower \( K^* \) (such as in local melt pod), \( \tilde{p}_r \) will have a less dramatic drop from \( \tilde{p}_0 \) than the kyanite case analyzed above. But in the local melting scenario, there are no viable mechanisms that an extremely high initial \( \tilde{p}_0 \) can be built. As melt-pressure facilitates melt-induced embrittlement (e.g., Brown and Solar, 1998), melt-generated \( \tilde{p}_0 \) must be limited by the brittle strength of the rock. This is supported by the commonly observed dispersed morphology of leucosomes in migmatites. We think it is unlikely that super-high melt-pressure can be built and sustained to cause UHP metamorphism as proposed by Vrijmoed et al. (2009).

We note that the above analysis, which was published in a journal article (Jiang and Bhandari, 2018), has been misrepresented in recent work by Moulas et al. (2020). The
authors wrote “…The large values of elastic moduli of minerals have been used to advocate that such stress differences would immediately dissipate since only small strains are required to relax a large pressure difference (Jiang and Bhandari, 2018, p. 406). There is a logical flaw in this line of reasoning; large elastic moduli are the cause of stress build up in the first place, hence they cannot, at the same time, be the cause of stress relaxation. If such arguments were true, it would have been impossible to measure any residual pressure/stress experimentally, since only a few percent of strain would have been sufficient to relax it. In order to calculate stress relaxation in host-inclusion systems, complete mechanical models with realistic rheologies should be used in a closed system of equations.” First, we point out that elastic moduli are neither the cause of stress/pressure buildup nor the cause of their relaxation. Instead, it is the change of loading conditions and the accompanying recovery of elastic strains that will affect the stress build-up and relaxation in the material. We never implied in our paper that large elastic moduli were the cause of stress/pressure relaxation. For a mineral grain with large bulk modulus $K$, it is an obvious fact that a small change in its volume strain $\Delta \varepsilon_v$ corresponds to a large change in pressure, as $\Delta p = -K \Delta \varepsilon_v$. Therefore, it is certainly true that if a strong phase is allowed to recover a small amount $\Delta \varepsilon_v$ through its interaction with the HEM, it will relax a large $\Delta p$. Second, in terms of “complete mechanical models with realistic rheologies”, our paper included a micromechanical Eshelby’s inhomogeneity problem as described above, which the authors seem to have missed. And finally, we again emphasize not to confuse the situation of a strong phase enclosed in a weak HEM (like a kyanite grain in a quartz-feldspathic matrix) with the case of a phase entrapped in a strong host mineral (like coesite in garnet). In the latter situation, the high pressure of the entrapped phase may be largely retained due to the high strength of the host mineral (pressure vessel effect) which prevents volume strain of the entrapped phase.

3.7 Comments on some field reports of high-pressure minerals

In recent literature, the concept of tectonic pressure has been invoked by some field investigations. Here, we briefly discuss some of these works, comment on the mechanical
feasibility of the ‘tectonic pressure’ concept in specific geological situations and point out key areas for future research.

Chu et al. (2017) applied diffusion modeling of chemical zonation in garnets to determine the P-T-t paths for the eclogite metamorphic assemblages from the Taconic orogenic belt, southern New England. These authors found the timescale for compression to eclogite facies to be \(\sim\)500 years, which if standard lithostatic pressure assumptions are applied, would mean descent rates too high to be explained by typical tectonic rates(<15cm/yr.). Hence, the authors invoked transient ‘tectonic pressure’ to explain the observed P-T-t path. Their interpretation correlates well with our work. As discussed above, the pressure deviations due to tectonic deformation are limited by the strength of the rocks and are in the levels of deviatoric stresses that the rock element can sustain. While deviatoric stresses for geological timescales (~Myr) are likely to be in ~MPa levels, short-term elastic interactions may cause high deviatoric stresses (~GPa levels) and hence high-pressure deviation for short-term timescales (ranging from ~100 years to thousand years). The short-term chemical diffusion process that recorded garnet zones was likely affected by tectonic pressure deviation for such short-timescale.

In a similar example from Monte Rosa tectonic unit, the Western Alps, Luisier et al. (2019) demonstrated using the field and microstructural observations, phase petrology, and geochemistry, that the observed pressure estimate variations from whiteschist to metagranite rock unit cannot be explained by tectonic mixing, retrogression of high-pressure minerals or lack of equilibration of mineral assemblages. The authors have therefore suggested tectonic pressure deviation due to high transient differential stresses (~1.4 GPa) as a possible explanation for the local pressure variation. The outcrop is also limited to few meters. We note, however, that there is no explicit evidence/information available for the timescale of the involved geological process (e.g., metasomatic alterations) responsible for mineral assemblages’ formation. Future studies obtaining P-T-t paths from such mineral assemblages can give a conclusive estimate of a short period for which transient tectonic pressure deviations might have been significant.
Cutts et al. (2020) applied Lu-Hf garnet geochronology along with the conventional thermobarometry for garnet-clinopyroxene-orthopyroxene assemblages to test the occurrence and magnitude of the tectonic pressure deviations in enstatite eclogite from Western Gneiss Complex (WGC), Norway. They found that the enstatite eclogite equilibrated at the time much later than the typical age of other eclogites from WGC and represents a time when the terrane was already at crustal depths (< 2.5 GPa). To reconcile this, the authors have invoked the tectonic pressure concept, which requires high transient differential stresses to generate high tectonic pressure deviations. Alternatively, this new age discovery of the enstatite equilibration may indicate a more complex history of exhumation as previously understood (Hacker et al., 2010). More investigations are required from the study area to get a conclusive estimate on P-T-t history.

There have been some field-based investigations that reported inconsistencies between the geothermobarometric pressure estimates and structural kinematic restorations (e.g., Nagel, 2008; Pleuger and Podladchikov, 2014; Schenker et al., 2015). These inconsistencies have been interpreted to indicate heterogeneously distributed pressure variations. If that is the case, it would require high deviatoric stresses (~GPa) at an orogenic scale to be maintained for geological timescales (~Myr), which seems highly unlikely. Short-term high deviatoric stresses could generate high transient pressure deviations leading to some rock records if suitable processes/mechanisms are available. A notable feature however in such records would be that the transient tectonic pressure is related to the spatial localization of the mineral assemblages. The high-pressure mineral assemblages from the field investigations should be re-evaluated in this context. Additional investigations involving the estimations of P-T-t paths (e.g., Chu et al., 2017) are required from such geological settings to confirm the timescales of geological processes responsible for such pressure records.

High rates of decompression in rocks can be reasonably explained by exhumation models involving trans-lithospheric diapirism, or buoyancy flow of melt pods (e.g., Cloos et al., 2005; Hacker, 2007; Little et al., 2011). It is the rates of compression an order of magnitude or faster than possible with tectonic burial, that is a critical test for the ‘tectonic over-pressure’ hypothesis. At present, such estimates of compression rates are
lacking from many field investigations that invoke tectonic pressure concepts (e.g., Pleuger and Podladchikov, 2014, Schenker et al., 2015). Future studies should be aimed at estimating the P-T-t paths for such high-pressure mineral assemblages. If a geological process forming mineral assemblages occurs at short-term timescales, tectonic pressure deviation might be significant and may get recorded locally. It is however very critical to emphasize that such imprint of transient tectonic pressure deviation is spatially localized, and there are UHP minerals over thousands of square kilometers (e.g., Dabie Shan and Western Gneiss) that are still explained by the conventional lithostatic pressure assumptions.

3.8 Conclusions

By regarding a representative volume element of Earth’s lithosphere as a composite material made of RDEs, we have shown that the pressure deviation in any RDE is below the deviatoric stress invariant in the macroscale HEM or the deviatoric stress invariant in the RDE itself. In relatively weak RDEs, the pressure deviation is unaffected by the power-law stress exponent. In relatively strong RDEs, the pressure deviation decreases as the power-law stress exponent increases. The pressure deviation in anisotropic viscous materials is lower than in isotropic materials.

Our prediction that the maximum pressure deviation is always below $\Sigma_{II}$ or $\sigma_{II}$ is directly testable by future metamorphic petrology studies. If a field area shows pressure variation across different RDEs and it can be demonstrated that post-metamorphism tectonic juxtaposition of RDEs is ruled out, then the maximum pressure variations should reflect the long-term deviatoric stress invariant in the area at the time of metamorphism. Future work is critical to clarify the actual level of pressure variation in rocks. P-T-t paths of the mineral assemblages can give a conclusive estimate if short-term high deviatoric stresses can record high-pressure deviations.

Local initial pressure perturbations are unlikely significant to cause long-term grain-scale pressure deviations because the initial pressure perturbations are either largely released by infinitesimal elastic volume strains or are hard to be sustained for long times.
3.9 References


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Chapter 4

4 A multiscale numerical modeling investigation on the significance of flow partitioning for the development of quartz c-axis fabrics

4.1 Introduction

Quartz c-axis fabrics are widely used to infer flow kinematics (e.g., Lister and Hobbs, 1980; Price, 1985; Simpson and Schmid, 1983) as well as deformation temperature (e.g., Faleiros et al., 2016; Law, 2014) and mechanisms (e.g., Schmid and Casey, 1986; Stipp et al., 2002) of ductile shear zones in Earth’s lithosphere. In terms of kinematics, the asymmetry of a c-axis fabric with respect to the shear zone coordinates is routinely used to infer sense of shear (e.g., Lister, 1977; Lister and Price, 1978; Lister and Williams, 1979; Menegon et al., 2008; Price, 1985). Fig. 4.1 summarizes the standard models for this practice (e.g., Passchier and Trouw, 2005). Note we have adopted the convention of Lister (1977) to present the c-axis fabrics whereby the shear plane (C-foliation) is vertical east-west and the shear direction (the Lc-lineation of Lin et al., 2007) is horizontal east. This convention differs from the one that orients the S-foliation east-west and Ls-lineation horizontal east (e.g., Passchier and Trouw, 2005). Natural quartz c-axis fabrics mainly comprise of single- and cross-girdles. In the coordinate system used here (Fig. 4.1), the cross-girdle has its dominant girdle normal to the shear plane, and the weaker girdle inclined antithetically to the shear sense (Fig. 4.1a). Single c-axis girdles either incline antithetically to the shear sense or are nearly normal to the shear plane (Fig. 4.1b, c). Point maxima within the girdles may lie at the periphery, the center, or intermediate positions between the periphery and the center. These are interpreted as reflecting the slip systems during deformation (e.g., Mainprice et al., 1986; Okudaira et al., 1995; Schmid and Casey, 1986; Simpson and Schmid, 1983). The models summarized in Fig.4.1 were based on numerical modeling of pure quartz aggregates using the Taylor-Bishop Hill model (e.g., Lister, 1977; Lister and Hobbs, 1980; Lister and Williams, 1979) and the viscoplastic self-consistent (VPSC) model (e.g., Morales et al., 2011; Nie and Shan, 2014; Wenk et al., 1989). Both model methods predicted that the c-axis girdle is
antithetic or normal to the shear zone boundary in the coordinate system used here. Modeling has never generated girdles synthetically inclined to the shear plane.

However, synthetically-inclined girdles have been observed in both natural shear zones (e.g., Keller and Stipp, 2011; Kilian et al., 2011, Law et al., 2010; Little et al., 2016) and creep experiments of quartz aggregates (e.g., Heilbronner and Tullis, 2006; Kilian and Heilbronner, 2017). Heilbronner and Tullis (2006) suggested that the synthetical orientation is due to rotation with vorticity of earlier antithetic girdles as finite strain increases. But this is not supported by any numerical modeling work with fairly large shear strains (up to 5, e.g., Jessell and Lister, 1990; Morales et al., 2011). Little et al (2016) suggested that general plane-strain flows may lead to synthetically-inclined c-axis girdles. The VPSC models of Takeshita et al. (1999) and Nie and Shan (2014) considered such flows but did not produce any synthetically-inclined c-axis girdles. However, their model did not consider cases where prism\textsuperscript{a} and rhomb\textsuperscript{a} slips are more significant than basal\textsuperscript{a} slip. Through VPSC modeling, Keller and Stipp (2011) produced synthetically-inclined c-axis girdle with rhomb\textsuperscript{a}, prism\textsuperscript{a}, and prism\textsuperscript{c} all active and all more significant than the basal\textsuperscript{a} slip system. However, there are natural samples with synthetically-inclined c-axis girdles (e.g., Little et al., 2016, Kilian et al., 2011; Law et al., 2010) that were produced in the temperature range ~350-550°C much below that required for the activation of prism\textsuperscript{c} slip (Toy et al., 2008). Furthermore, c-axis fabrics with both synthetically- and antithetically-inclined c-axis girdles have been observed in the same thin section (Kilian et al., 2011 their fig. 8, 9). Therefore, it is important to clarify if the combination of rhomb\textsuperscript{a} and prism\textsuperscript{a} slip, without prism\textsuperscript{c}, can generate these synthetically-inclined c-axis girdles.
The standard models summarized in Fig. 4.1 are based on the deformation of pure quartz aggregates under limited (mostly simple shearing) single-scale uniform flows (e.g., Lister et al., 1978; Lister and Hobbs, 1980; Lister and Williams, 1980; Keller and Stipp, 2011; Morales et al., 2014; Nie and Shan, 2014; Wenk et al., 1989). The spatial variation of quartz c-axis fabrics is a manifestation of heterogeneous deformation and, we suspect, is related to flow partitioning (e.g., Jiang, 1994a, 1994b; Lister and Williams, 1983) and strain buildup in rheologically distinct domains. Most natural mylonites are made of polyphase minerals in which the microscale rheology varies from one domain to another which facilitates flow partitioning. Many authors have referred to flow partitioning qualitatively (e.g., Killian et al., 2011; Garcia Celma, 1982; Jerabek et al., 2007; Larson et al., 2014; Law, 1987; Lister and Price, 1978; Passchier, 1983; Pauli et al., 1996; Peternell et al., 2010) to explain observed c-axis fabric variations.

Figure 4.1: Current models for interpreting quartz c-axis fabrics at low to medium temperatures ~350-550°C presented in the shear zone coordinate system. The sense of shear is dextral. Cross-girdle and single girdle c-axis fabrics are commonly observed. (a) c-axis cross girdle pattern with one girdle normal to the shear plane while the other antithetic to the shear sense. (b) a single c-axis girdle with Y-maxima, inclined either antithetically to the shear sense or normal to the shear plane. (c) a single c-axis girdle inclined either antithetically to the shear sense or normal to the shear plane. The c-axes near the periphery, the center, and in between are interpreted to reflect basal, prism, and rhomb slips respectively.
In this contribution, we apply a multiscale numerical modeling approach to quantitatively investigate the consequence of flow partitioning on the development of quartz c-axis fabrics and compare our modeling results with natural and experimental observations. Specifically, we use the mylonite thin-section photomicrograph of Killian et al. (2011, Fig.8 there) as a model and seek to understand if flow partitioning can produce the observed variation in quartz c-axis fabrics.

4.2 Approach

Fig.4.2a shows the thin-section photomicrograph from Kilian et al. (2011). The rock is comprised of quartz domains (from which c-axis fabrics were presented), feldspar porphyroclasts, and a matrix of fine-grained quartz, feldspar, and mica. According to Kilian et al. (2011), the microstructure was produced in a simple shearing flow which is consistent with the geometric pattern of the foliation (Ramsay, 1980; Ramsay and Graham, 1970). In this investigation, we consider plane-strain general shearing flows as the bulk flow field to understand how the partitioning of a given bulk flow into rheologically distinct quartz domains may affect the c-axis fabrics in those domains. Our method here, however, also applies to any 3D general shearing flows (e.g., Jiang and Williams, 1998).

In the coordinate system used in this investigation (Fig. 4.2c), a general plane-strain general shearing flow is defined by the following Eulerian velocity gradient tensor:

\[
L = \begin{pmatrix}
\dot{\varepsilon} & \dot{\gamma} & 0 \\
0 & -\dot{\varepsilon} & 0 \\
0 & 0 & 0
\end{pmatrix}
\] (4.1)

where \( \dot{\gamma} (\dot{\gamma} > 0) \) is the shear strain rate for the simple shearing component and \( \dot{\varepsilon} (\dot{\varepsilon} > 0) \) is the strain rate parallel to the X-axis. The flow in Eq. 4.1 corresponds to a kinematic
Figure 4.2: Illustration of the multiscale approach used in this paper. (a) The thin section photomicrograph of a natural mylonite from Kilian et al. (2011) used as a model. (b) Sketch of (a). The thin section can be viewed as a 2D section of the representative volume element (RVE) for the shear zone material, which is composed of quartz domains, feldspar porphyroclasts, and mica seams in a fine-grained matrix. The quartz domains and feldspar clasts are referred to as Rheologically Distinct Elements (RDEs). We are concerned with partitioned flows in quartz RDEs in this paper. (c) Coordinate system to define the macroscale flow field used in modeling investigation (d) Each quartz RDE is regarded as a heterogeneous Eshelby inclusion embedded in the composite shear zone material that is idealized as the Homogeneous Equivalent Matrix (HEM). Microscale fields (strain rate $\varepsilon$, and vorticity $w$) are related to respective macroscale fields ($E$ and $W$) by partitioning equations, where $A$ is the strain rate partitioning tensor, $S$ and $\Pi$ are respectively the 4th-order symmetric and anti-symmetric Eshelby tensors (Jiang, 2014).
vorticity number \( W_k = \frac{\dot{\gamma}}{\sqrt{4\varepsilon^2 + \dot{\gamma}^2}} \) (Jiang and White, 1995; Li and Jiang, 2011; Truesdell, 1953). We consider the variation of the flow by varying \( W_k \) from 0 to 1.

The progression of the finite strain is measured by a strain intensity defined as \( \rho = \sqrt{\left( \ln \frac{s_1}{s_2} \right)^2 + \left( \ln \frac{s_2}{s_3} \right)^2} \) where \( s_1, s_2, s_3 \) are the three principal stretches \( (s_1 > s_2 > s_3) \) of the finite strain ellipsoid (e.g., Yang et al., 2019). In the event of simple shearing \( (W_k = 1) \), the strain can also be measured by the shear strain \( \dot{\gamma} \). The relation between \( \dot{\gamma} \) and \( \rho \) in the simple shearing situation is shown in Fig. 4.3.

![Figure 4.3: The macroscale finite strain of the shear zone, measured by the strain intensity \( \rho \), as a function of shear strain \( \dot{\gamma} \) in simple shear case \( (W_k = 1) \).](image-url)
We use the Viscoplastic-Self-Consistent (VPSC) model, originally due to Molinari et al. (1987) and further developed by Lebensohn and Tome (1993), to simulate the quartz c-axis fabric development in a flow field. Specifically, VPSC7 (Lebensohn and Tomé, 2009) for Windows is used in this investigation. We track the c-axis evolution of 500 quartz crystals whose initial orientations are randomly distributed in 3D space (Jiang 2007b). The initial shapes of grains are equant. The crystal shapes evolve with strain and the grain fragmentation scheme of Beyerlein et al. (2003) is used to limit the aspect ratio of quartz grains to mimic some effect of dynamic recrystallization. The VPSC output of c-axis data is plotted using the MTEX toolbox (Bachmann et al., 2010). Since we are concerned with variation in quartz c-axis fabrics, we present pole figures of the (0001) directions here. Pole figures of other crystal directions are provided in the supplementary material (download link provided in Appendix F).

The relative activity of slip systems is modulated in VPSC by their relative critical resolved shear stress (CRSS). A lower CRSS corresponds to higher activity. For quartz, the CRSS for a slip system is largely temperature-dependent with basal <a> slip occurring at about 350-500°C, rhomb<a> and prism<a> slip at ~ 500-600°C, and prism<c> slip at >650°C (e.g., Toy et al., 2008). Table 4.1 summarizes the slip system combinations used in this study based on previous work (e.g., Lister and Paterson, 1979; Morales et al., 2014; Wenk et al., 1989). They are labelled as Model-A to F. Morales et al (2014) and Keller and Stipp 2011) made a distinction between rhomb (+) slip{r} in <a> direction and rhomb (-) slip{z} in <a> direction in their modelling works. This distinction may be important in regime 1 dislocation creep (Hirth and Tullis, 1992) but it is not necessary for our work here on the effect of flow partitioning.
In the single-scale case, the flow field defined in Eq. 4.1 is used in the VPSC directly for the simulation of the resulting quartz c-axis fabric development. In the multiscale case, Eq. 4.1 defines the bulk macroscale flow which must be partitioned into different rheologically distinct quartz domains (Figs. 4.2b and d) before the quartz c-axis fabric development in those domains can be simulated with VPSC. We use the self-consistent Multi Order Power Law Approach (MOPLA) (Jiang and Bentley, 2012; Jiang, 2016, 2014; Qu et al., 2016; and Lu, 2020) to obtain the partitioned flow fields in quartz domains. The multiscale approach can be illustrated using the thin section sample in Fig.4.2a as follows: Quartz domains, feldspar porphyroclasts, and mica seams are referred to as Rheologically Distinct Elements (RDEs). The sample as a whole was subjected to a macroscale flow field like Eq. 4.1. In micromechanics terms, the macroscale flow is the bulk flow averaged on a Representative Volume Element (RVE) which represents the mineral assemblage for the sample. It is reasonable to regard the thin section as a section of the RVE for the macroscale flow. The microscale flow field in each constituent RDE such as a quartz domain is distinct and differs from the macroscale flow because each RDE is unique in its rheology, shape, and orientation (Eshelby, 1957; Mura, 1987; Jiang 2014, 2016). Clearly, it is the microscale (or partitioned) flows in quartz domains that are responsible for the quartz c-axis fabric development.

In MOPLA, an RDE is regarded as an ellipsoidal Eshelby inhomogeneity embedded in and interacting with the macroscale material (Fig. 4.2d). The rheology of the latter is

<table>
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<tr>
<th>Slip Systems</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
</tr>
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<tbody>
<tr>
<td>Basal &lt;a&gt; {0001} &lt;12\bar{1}0&gt;</td>
<td>1</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>Rhomb &lt;a&gt; {10\bar{1}1} &lt;1\bar{2}1\bar{0}&gt;</td>
<td>5</td>
<td>5</td>
<td>1</td>
<td>1</td>
<td>5</td>
<td>3</td>
</tr>
<tr>
<td>Prismatic &lt;a&gt; {10\bar{1}0} &lt;1\bar{2}1\bar{0}&gt;</td>
<td>5</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>Prismatic &lt;c&gt; {10\bar{1}0} &lt;0001&gt;</td>
<td>10</td>
<td>10</td>
<td>10</td>
<td>10</td>
<td>1</td>
<td>1</td>
</tr>
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Table 4.1: Quartz slip systems and the relative CRSS values for different models used in VPSC simulation.
approximated by a homogeneous effective medium (HEM) and obtained from the rheologies of the constituent RDEs from a set of homogenization equations. The microscale or partitioned flows in an RDE are related to the macroscale flow, which is assigned by Eq. 4.1, by a set of partitioning equations (for details, see Jiang 2014, 2016). The partitioning and homogenization equations are solved simultaneously to obtain the partitioned flow fields and the macroscale rheology. As the relevant rheology for mylonites is power-law viscous (Kohlstedt et al., 1995), the MOPLA formulation adopts a linearization approach (Lebensohn and Tomé, 1993; Molinari et al., 1987) where linearized viscosities such as tangent viscosities are used in the formulation. As we are concerned with quartz c-axis fabric development, we specifically use MOPLA to calculate the partitioned flow fields within quartz domains.

We consider two situations for the rheology of the quartz RDEs and HEM. In the first, both the RDEs and the HEM are isotropic. The rheological contrast between an RDE and the HEM is reduced to an effective viscosity ratio \( r \) between the RDE to the HEM. We do not consider the rheological anisotropy development in HEM as a result of fabric buildup with strain because the anisotropic rheological response of the constituent RDEs is not available. Because of power-law rheology, \( r \) varies with time. We thus consider a range of constant \( r \) values. The quartz aggregates in Fig. 4.2a all have convex shapes with surrounding matrix material wrapping around them, suggesting that quartz RDEs were rheologically stronger \((r > 1)\) than the ambient HEM. But \( r \) cannot be too high (e.g., \( r > 10 \)) because of power-law rheology or the quartz RDEs would behave like rigid clasts (Jiang, 2007b; Xiang and Jiang, 2013) with no c-axis fabric formation. We consider the situations of \( r \) being 2, 5, and 10. The situation of \( r = 0.5 \) is also considered here for comparison to show what the c-axis fabrics might be like if quartz RDEs were mechanically weaker than the ambient medium.

In the second situation, we consider isotropic RDEs in a HEM of simple planar anisotropy which approximates a foliated and/or layered material like natural mylonites. The rheology of such a HEM can be characterized by two distinct viscosities: \( \eta_n \), the normal viscosity for the resistance to pure shearing along and perpendicular to the
layering, and \( \eta \) the shear viscosity measuring the resistance to shearing parallel to the layering (e.g., Jiang, 2016; Fletcher, 2009; Johnson and Fletcher, 1994). The strength of anisotropy is measured by the ratio \( m \) of \( \eta \) to \( \eta_b \). For foliated and layered rocks, \( m > 1 \) (Treagus, 2003). The rheological contrasts between the isotropic quartz RDE and HEM can be defined by the following two parameters: the ratio, \( r_{\text{eff}} \), between the viscosity of the RDE to \( \eta_b \) and \( m \). In such a case, the effective viscosity of the RDE is simply given by \( r_{\text{eff}} \eta_b \). Similar to the isotropic cases, we consider \( r_{\text{eff}} \) being 0.5, 2, 5, and 10. Fig. 4.4 shows the geometric relation between the flow field and the plane of anisotropy. Macroscale flow is simple shear with shear plane parallel to X-Z plane.

\[
m = \frac{\eta_s}{\eta_b}
\]

**Figure 4.4: Geometric relation between the macroscale flow field and anisotropy plane in the planar anisotropic HEM.**

To cover the shape variation of quartz RDEs, we considered three reference initial shapes: prolate (5:1:1), oblate (5:5:1), sphere (1:1:1), and initial triaxial RDEs with long and short semi-axial length fixed to 5 and 1 respectively and intermediate semi-axial length ranging from 2-4. These initial RDEs will deform into various possible triaxial shapes in nature. The initial orientations of the RDEs are defined by spherical angles (Jiang, 2007a, b) which are randomly assigned.
The partitioned flow for a quartz RDE computed from MOPLA is used as the input flow field to simulate the quartz c-axis fabrics in that RDE through the VPSC model. Because the partitioned flow field in any given RDE is non-steady as the RDE continuously changes shape and orientation during deformation, the coupled computation between MOPLA and VPSC is carried out as follows: With a given macroscale flow field defined in Eq. 4.1, we use the MOPLA algorithm implemented in MATLAB (Lu, 2020; Jiang, 2016, 2014, 2007a; Jiang and Bentley, 2012; Qu et al., 2016) to calculate the partitioned flow in every quartz RDE, which is expressed as a velocity gradient tensor. We export to a data file the RDE velocity gradient tensor for every prescribed macroscale strain increment until a pre-set macroscale finite strain is reached. This data file is then used as input flows into the VPSC code to calculate the c-axis fabric evolution within the RDEs as macroscale strain increases until the set magnitude. The velocity gradient tensor files for all the RDEs are available in the supplementary material.

4.3 Results

As mentioned above, we have simulated quartz c-axis fabric development in three situations. The first is in homogeneous macroscale plane-strain general shearing flows, without flow partitioning, with quartz slip system combinations that have not been covered by previous studies. The second situation is when rheologically distinct quartz domains are within an isotropic HEM, and the third is when the quartz domains are within a HEM of planar anisotropy.

4.3.1 Quartz c-axis fabric development in homogeneous plane-strain general shearing flows

Figs. 4.5 and 4.6 present quartz c-axis fabrics produced for models-A-F (rows) under uniform macroscale flows of plane-strain general shearing from $\kappa_W = 0$ to $\kappa_W = 1$ (columns), at macroscale strain states $\rho = 2$ and 6.

In pure shearing ($\kappa_W = 0$), for models-A, C, and D, peripheral c-axis maxima form and remain at the maximum shortening direction regardless of strains (Figs. 4.5a,d, m,p, 4.6a,d). For model-B, a cross-girdle (Figs 4.5g) form at $\rho = 2$, with its central segment
lying along the maximum shortening direction. A single girdle is produced lying along the maximum shortening direction (Figs. 4.5j) at $\rho = 6$. For models-E and F, peripheral maxima develop and remains at the maximum stretching direction at both strain states (Figs. 4.6g, j, m, p).

When $0 < W'_k \leq 1$, for models-A, C, and D and at $\rho = 2$, peripheral c-axis maxima are developed inclining antithetically to the shear sense (Figs. 4.5b, c, n, o, 4.6b, c). As $W'_k$ increases, the angle between the peripheral c-axis maxima and the shear plane normal increases. The peripheral maxima rotate with macroscale vorticity as finite strain increases but do not pass the shear plane normal (Figs. 4.5f, l, q, r, 4.6f). For model-B, a cross-girdle, with its central segment lying normal to the shear plane, is formed at $\rho = 2$ (Figs 4.5 h, i). At $\rho = 6$, this cross-girdle becomes a single girdle lying normal to the shear plane (Figs. 4.5 k, l). In some general shear ($0 < W'_k < 1$) cases, the c-axis girdles can be slightly synthetically-inclined at $\rho = 6$ (Figs. 4.5e,k, 4.6e), but the angle between the peripheral c-axis maxima and the shear plane normal is small ($< 10^\circ$). For models-E and F, the c-axis peripheral maxima are synthetically-inclined near the shear direction at $\rho = 2$. The angle between the peripheral c-axis maxima and the shear direction increases with $W'_k$ (Figs. 4.6h, i, n, o). The c-axis peripheral maxima rotate with vorticity toward the shear direction as the finite strain increases (Figs. 4.6 k, l, q, r).
Figure 4.5: C-axis fabrics in single-scale deformation with varying $W_k$ from pure shearing to simple shearing and for models-A-C. The final strain intensity is between $\rho = 2$ and 6. The pole densities are contoured in multiples of uniform distribution as shown in the color bar.
Figure 4.6: Same as Figure 4.5 but for models -D-F.
4.3.2 Quartz c-axis fabric development in quartz domains embedded in an isotropic HEM

Since models-A, B, C, and D all produce similar c-axis fabrics with c-axis girdles antithetically-inclined or nearly normal to the shear plane, we only present results for model-A for multiscale deformation. Figs. 4.7 and 4.8 reports ten results of c-axis fabrics produced in quartz RDEs of varying initial shapes, orientations, and viscosity ratio $r$ under a range of macroscale flow fields. These results can be summarized as follows: When $0 < W_k \leq 1$, c-axis girdles are always antithetically-inclined (Figs. 4.7a, b, d, e, g, h, j, k, m, n, 4.8a, g, j, m) regardless of initial conditions of RDEs up to the finite strain $\rho \sim 4$. With an increase in finite strain, the girdles rotate with bulk vorticity (rows of Figs. 4.7 and 4.8) but do not pass the shear plane normal unless $r \geq 5$ (Figs. 4.7-i, l, o, 4.8-b, c, i, l, o). If the RDEs were weaker than the HEM ($r = 0.5$), c-axis girdles remain normal (Figs. 4.7-c) to the shear plane even at very high finite strains ($\rho \sim 6-7$). In pure shearing, a cross girdle is produced at $\rho \sim 2$ which becomes a single girdle at $\rho \sim 6$ with peripheral c-axis maxima always parallel to the maximum shortening direction (Figs. 4.8-d, e, f).

4.3.3 Quartz c-axis fabric development in quartz domains embedded in a planar anisotropic HEM

Figs. 4.9a-o report c-axis fabrics developed in quartz RDEs of varying initial shapes, orientations, and viscosity ratio $r_{eff}$, embedded in a planar anisotropic HEM of anisotropic strength $m$ as described in Section-4.2. These results can be summarized as follows: The c-axis girdles are always antithetically-inclined (Figs. 4.9a, d, g, j, m) at $\rho \sim 2$ regardless of $W_k$, $r_{eff}$, $m$, initial orientations and shapes of RDEs. The girdles rotate with bulk vorticity as $\rho$ increases (rows of Figs. 4.9) but do not pass the shear plane normal unless $r_{eff} \geq 2$ (Figs. 4.9 i, l, o). If RDEs were weaker ($r_{eff} = .5$), c-axis girdles are close to normal (Figs. 4.9c, f) to the shear plane even at high finite strains ($\rho \sim 6-7$).
Figure 4.7: C-axis fabrics in selected quartz RDEs in an isotropic HEM under simple shearing ($W_k = 1$). (a)-(o) are the resultant c-axis fabrics developed. The first column presents the initial conditions for the RDEs [ $r$ : viscosity ratio of the RDE to HEM, initial shape defined by semi-axes of the RDE ($a_1 : a_2 : a_3$, where $a_1 \geq a_2 \geq a_3$), and initial orientation given by spherical angles ($\theta_1$, $\Phi_1$, $\theta_2$) for general RDEs or ($\theta$, $\Phi$) for spheroidal RDEs]. Each row presents the results for the RDE as the macroscale strain increases.
\begin{figure}
\centering
\begin{tabular}{|c|c|c|c|}
\hline
\begin{tabular}{c}
$W_k=1,$ \\
$r=8,$ \\
$5:3:1,$ \\
$(0,90,0)$
\end{tabular} & \begin{tabular}{c}
$\rho=4.5$
\end{tabular} & \begin{tabular}{c}
$\rho=6.5$
\end{tabular} & \begin{tabular}{c}
$\rho=6.8$
\end{tabular} \\
\hline
\begin{tabular}{c}
$W_k=0,$ \\
$r=5,$ \\
$5:3:1,$ \\
$(0,0,135)$
\end{tabular} & \begin{tabular}{c}
$\rho=2$
\end{tabular} & \begin{tabular}{c}
$\rho=4$
\end{tabular} & \begin{tabular}{c}
$\rho=6$
\end{tabular} \\
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\begin{tabular}{c}
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$r=5,$ \\
$5:1:1,$ \\
$(0,0)$
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$\rho=2$
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$\rho=4$
\end{tabular} & \begin{tabular}{c}
$\rho=6$
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\hline
\begin{tabular}{c}
$W_k=0.75,$ \\
$r=5,$ \\
$5:1:1,$ \\
$(135,90)$
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\end{tabular} & \begin{tabular}{c}
$\rho=4$
\end{tabular} & \begin{tabular}{c}
$\rho=6$
\end{tabular} \\
\hline
\begin{tabular}{c}
$W_k=0.9,$ \\
$r=5,$ \\
$5:5:1,$ \\
$(0,0)$
\end{tabular} & \begin{tabular}{c}
$\rho=2$
\end{tabular} & \begin{tabular}{c}
$\rho=4$
\end{tabular} & \begin{tabular}{c}
$\rho=6$
\end{tabular} \\
\hline
\end{tabular}
\caption{Same as Figure 4.7 except that the macroscale flow is plane strain general shearing ($0<W_k\leq1$).}
\end{figure}
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<tbody>
<tr>
<td>(a)</td>
<td>(b)</td>
<td>(c)</td>
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<td>(d)</td>
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<td>(m)</td>
<td>(n)</td>
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Figure 4.9: C-axis fabrics in selected quartz RDEs in a HEM with planar anisotropy under simple shearing flow ($W_k = 1$) (a)-(o) are the resultant c-axis fabrics developed. The first column presents the initial conditions for the RDEs [$r_{\text{eff}}$ - viscosity ratio of the RDE to HEM’s $\eta_k$, initial shape defined by semi-axes of the RDE ($a_1:a_2:a_3$, where $a_1 \geq a_2 \geq a_3$), initial orientation given by spherical angles ($\theta_1$, $\Phi_1$, $\theta_2$) for general RDEs or ($\theta$, $\Phi$) for spheroidal RDEs, and anisotropic strength $m$]. Each row presents the results for the RDE as the macroscale strain increases.
4.4 Discussion

In Section 4.2, we argued that \( r \) must be greater than 1 from microstructures (Fig. 4.2a) but not so high that the quartz RDEs do not develop enough internal strain for c-axis fabric formation. In our modeling, we considered the range \( r \) between 2 and 10. Our modeling results show that, with basal\(<a>\), rhomb\(<a>\), and prism\(<a>\) slips, c-axis girdles in a quartz RDE always develop at an antithetical orientation initially. But the girdles rotate with vorticity as the macroscale finite strain increases. If the RDE is sufficiently strong (in isotropic HEM case and \( r_{\text{eff}} \geq 2 \) in planar anisotropic HEM case), the girdles will rotate past the shear zone normal and lie in the synthetical sector at high strains (\( \rho \sim 6 \), Figs. 4.7-i, 1, o, 4.8-b, c, i, l, o, 4.9-i, l, o). Our modeling results show that for synthetically-inclined girdles, \( r \) should be between 5 and 10. These results are consistent with the strain gradient of the thin section (Fig. 4.10, based on Killian et al., 2011, Fig.9 there). The antithetically-inclined c-axis peripheral maxima (yellow in Fig. 4.10) correspond to a lower strain and synthetically-inclined c-axis peripheral maxima (red in Fig. 4.10) to a higher strain.

Despite the variability of the partitioned flow field in quartz RDEs, we found out that the microscale vorticity in every quartz RDE still has the same sense as the macroscale vorticity. Fig. 4.11 shows the dot product of the unit vector \( \hat{\omega} \) parallel to the vorticity in an RDE and the unit vector \( \hat{\Omega} \) parallel to the macroscale vorticity. \( \hat{\omega} \cdot \hat{\Omega} \) is positive for all quartz RDEs (a few selected ones are shown in Fig. 4.11). In other words, there is no vorticity sense reversal in any quartz RDEs. This implies that the volume-weighted average of microscale vorticity vectors is parallel to the macroscale vorticity vector. Therefore, the c-axis vorticity axis (CVA) analysis (Giorgis et al., 2017; Michels et al., 2015) can still be used in every quartz RDE, and then the averaged microscale vorticity axes represent the macroscale vorticity axis.
Figure 4.10: Sketch of the thin-section sample showing c-axis fabric variation in quartz domains from Fig. 9 of Kilian et al (2011). C-axis fabrics comprise of peripheral c-axis maxima that are antithetically-inclined (yellow), nearly normal (blue), and synthetically-inclined (red) to the shear plane. The sense of shear is dextral. The arrow at the top-left shows the direction of increase in strain gradient.
Figure 4.11: Plot of dot product $\hat{\omega} \cdot \hat{\Omega}$ with increasing macroscale strain $\rho$, for 50 RDEs with random initial shapes and orientations, $r = 0.5, 2$ and $5$ (rows) and $W_k = 1$ and $0.75$ (columns). As defined in the text, $\hat{\omega}$ and $\hat{\Omega}$ are, respectively, the unit vectors parallel to the microscale vorticity vector in an RDE and the macroscale vorticity vector. $\hat{\omega} \cdot \hat{\Omega}$ is close to unity for the RDEs. Therefore, the microscale vorticity vectors are always of the same sense as and nearly parallel to the macroscale vorticity vector.
Synthetically-inclined c-axis girdles have also been reported in some creep experiments on pure quartz aggregates with similar slip systems (basal<\textit{a}>, rhomb<\textit{a}>, and prism<\textit{a}>) at high finite strains (Heilbronner and Tullis 2002, 2006). Although Keller and Stipp (2011) obtained synthetically-inclined c-axis girdles by including prism<\textit{c}> slip in their VPSC models, we have further confirmed that without prism <\textit{c}> slip (our model-D), synthetically-inclined c-axis girdles cannot be produced (Figs. 4.5a-f), unless flow partitioning is considered. We suspect that some degree of heterogeneous strain and therefore partitioned flow was responsible for such c-axis girdle orientations. Heilbronner and Tullis (2006) themselves suggested that different domains of polycrystal aggregates might exhibit different viscosities, which could have facilitated partitioning of the flow among different domains.

Li and Jiang (2011) raised issues with the practice of vorticity estimation using rigid porphyroclasts under the assumption of steady-state homogeneous flow histories. The significance of flow partitioning as demonstrated by our modeling based on microstructures of natural mylonites raises further issues with using quartz c-axis fabrics to estimate the (macroscale) vorticity (e.g., Vissers, 1989; Wallis, 1995, 1992; Xypolias, 2009; Law, 2010). First, where quartz c-axis fabrics have resulted from partitioned flow, the steady-state flow assumption is invalid. As we have shown, there is a distinct microscale vorticity history, not a constant vorticity number, in every quartz RDE, which cannot be determined from the final c-axis fabrics. In principle, the microscale vorticity in a quartz RDE does not have a simple relation to the macroscale vorticity. Second, even for the single-scale case where no flow partitioning is considered, our modeling demonstrates that the assumption commonly used in vorticity determination that the dominant c-axis girdle is perpendicular to the shear plane is not always valid.

Peripheral c-axis maxima close to the shear direction have commonly been taken to reflect prism <\textit{c}> slip (Passchier and Trouw, 2005). Our modeling suggests that they can also be significantly rotated peripheral basal <\textit{a}> maxima from certain quartz RDEs (Fig.4.8c). Larson et al (2014) have reported a possible example of this. They presented peripheral c-axis maxima close to the shear direction in a temperature condition much
below that required for the activation of prism <c> and used the concept of flow partitioning to explain their observation. Our modeling lends support to this explanation.

4.5 Conclusions

The co-existence of both synthetically-inclined and antithetically-inclined quartz c-axis girdles in a single thin section can be explained by flow partitioning at the thin section scale. The antithetically-inclined girdles correspond to relatively low finite strains and the synthetically-inclined girdles to high finite strains.

Although the microscale flow fields vary from one quartz RDE to another and are distinct from the macroscale flow, the sense of vorticity in every quartz RDEs remains the same as the macroscale vorticity.

Because of flow partitioning, it is not possible to estimate the vorticity number of the macroscale flow from quartz c-axis fabrics. But it is still possible to obtain the macroscale vorticity axis by averaging the microscale vorticity axes from quartz RDEs. The latter can be obtained through the c-axis vorticity axis analysis.

As a result of partitioned flows, the dominant quartz c-axis girdle can lie antithetical, normal, synthetical to the shear plane. The basal <a> peripheral maxima may end up lying close to the shear direction at high macroscale strains. Caution should be taken not to misinterpret these peripheral maxima as reflecting prism< c> slip.
4.6 References


Chapter 5

5 A micromechanics-based numerical modeling investigation on 3-D flanking structures and its application.

5.1 Introduction

Flanking structures are deflections in linear and planar fabric elements surrounding a rheological heterogeneity, also known as the cross-cutting element, such as a fracture, vein, dykes, or boudins. They are widely used by structural geologists to infer useful information such as finite strain magnitude, shear sense, and bulk flow type (Grasemann et al., 1999; Passchier, 2001; Kocher and Mancktelow, 2005). Correct interpretations of these structures are essential for understanding regional tectonics. Extensive analog and numerical modeling investigations have been carried out over the last few years (e.g., Grasemann and Stuwe, 2001, Grasemann et al., 2003; Wiesmayr and Grasemann, 2005; Exner et al., 2004; Exner and Dabrowski, 2010; Grasemann et al., 2010; Kocher and Mancktelow, 2005; Kocher and Mancktelow, 2006; Mulchrone, 2007) to understand the formation of flanking structures. However, the majority of these investigations assume cutting elements as a frictionless slip surface regarded as an inviscid material (e.g., Grasemann et al., 2003; Kocher and Mancktelow, 2005). In nature, the rheology of the cutting element can vary widely (Fig. 5.1). Only Grasemann and Stuwe (2001) and Mulchrone (2007) considered the cases of flanking structures around cutting elements with more variable rheological contrast to the embedding medium. Grasemann and Stuwe (2001) used a 2-D finite element modeling approach which was limited to low finite strain deformation ($\gamma = 2$), specific aspect ratio (10:1), and initial orientation (135° to the shear zone boundary) of the cutting element. Their model predicts only n-type flanking structures with ‘no offset’ along with a cutting element rheologically stronger than the embedding medium. However, there is evidence of natural flanking structures (e.g., Gayer et al., 1978; Mukherjee, 2014; Mukherjee and Koyi, 2009; Rice, 1986) where cutting elements rheologically stronger than the embedding medium may display some offsets. Clearly, where the cutting element is not rigid, it can deform and develop offsets,
even being rheologically stronger than the embedding medium. Mulchrone (2007) used an analytical solution for mechanical fields around a 2-D elliptical inclusion embedding in a viscous medium to simulate flanking structures up to high finite strains ($\gamma = 4$). They showed that ‘synthetic’ offsets can develop for a specific case of cutting element with viscosity 1.3 times the medium’s viscosity. However, their analysis is limited to a specific aspect ratio (50:1) and hence hard to apply on the natural examples of more varied shapes of cutting elements.

Recently, a new class of flanking structures, termed ‘Flanking Microstructures’ (Mukherjee, 2014; Mukherjee and Koyi, 2009) have been observed, that mainly comprise mineral inclusions as the cutting element. Such flanking structures cannot be understood using the previous models which are limited to high aspect ratio cutting elements corresponding to a slipping surface. An example includes a flanking microstructure reported by Mukherjee and Koyi (2009) from the Higher Himalayan Crystalline units, which shows a feldspar grain acting as a cutting element, deflecting the surrounding muscovite cleavage planes (their fig. 3c). In another example, Grasemann et al. (2011) and Exner and Dabrowski (2010) discovered some 3-D flanking structures that cannot be modeled using any available 2-D investigations (their fig. 1). Exner and Dabrowski (2010) used the limiting case of Eshelby solution (Eshelby 1957, 1959) for a 2-D elliptical crack of inviscid material to simulate flanking structures in 3D and showed that the 3-D model results in smaller offset across the cutting element than predicted with 2-D models. How the flanking structures may vary in 3-D for a cutting element with more variable rheological contrast is not known.
Figure 5.1. Examples of natural flanking structures (a) Flanking fold around a crack (red dots) from the Cross-lake group in Cross lake greenstone belt, Manitoba. Compositional layering forms the host element that gets deflected in the vicinity of the crack. (b) Flanking structure around slipping surfaces (red dots) from the Cap de Creus shear zone, Spain. Transposition foliation forms the host element that gets deflected in the vicinity of slip-surface. (c) Flanking folds around cross-cutting quartz veins from the Cross-lake group in Cross lake greenstone belt, Manitoba. Compositional layering forms the host element that gets deflected in the vicinity of the veins. Dotted lines represent the cutting element in each example (Photo courtesy of Dazhi Jiang).
In this work, we have applied the Exterior Eshelby solution for 3-D viscous inclusions (Jiang, 2016) to simulate flanking structures around a 3-D cutting element and demonstrate how flanking structures may vary with rheological contrast of the cutting element to the medium, initial shape, and orientation of the cutting element, 3-D geometry and finite strains. We reproduced all observed flanking structure types recognized from natural shear zones. In contrast to the previous models with limited cutting element geometry and rheological properties, our modeling results show that all three types of flanking structures with antithetic (a-type), no- (n-type), and synthetic (s-type) slip along the cutting element can be formed around any cutting element stronger than the embedding medium. The a-type flanking structure may transition into an s-type depending on the cutting element’s viscosity and macroscale finite strain. We have further developed a reverse-dynamic modeling tool that can provide a quantitative estimate of flow vorticity, finite strain, and cutting element’s viscosity relative to the embedding medium from an observed natural flanking structure.

5.2 A micromechanics-based model for simulating flanking structures

We use the general Eshelby formalism for a viscous ellipsoidal inclusion (Jiang, 2016, 2014, Lebensohn et al., 1998) to simulate flanking structures. The solution comprises partitioning equations that relate the local fields inside and around the inclusion (strain rate $\varepsilon$, vorticity $w$ ) to their respective far-field counterparts in the embedding medium (Fig. 5.2). The mechanical fields inside the ellipsoidal inclusions (interior fields) are constant while the fields around the inclusion (exterior) fields vary spatially with the position vector. These partitioning equations were derived for linearly viscous materials only. For power-law viscous materials such as rocks in the lithosphere (Kohlstedt et al., 1995), a linearization approach (e.g., Jiang, 2016, Lebensohn and Tome, 1993) can be applied. In such a case, a linearized viscosity such as the tangent viscosity (e.g., Jiang and Bentley, 2012) is used in these equations.
We regard any rheological heterogeneity (or cutting element in terms of flanking structure terminology) as an ellipsoidal inclusion, and partitioning equations allow the calculation of velocity gradient fields inside and around the heterogeneity, given by Eulerian velocity gradient tensors, as follows:

\[
L = \varepsilon + w \quad \text{(5.1a)}
\]

\[
L(x) = \varepsilon(x) + w(x) \quad \text{(5.1b)}
\]

Figure 5.2 Eshelby inclusion problem of an ellipsoidal viscous inclusion embedded in an infinite homogeneous viscous medium. \( \varepsilon \) and \( w \) are the uniform strain rate and vorticity fields inside the inclusion. \( \varepsilon(x) \) and \( w(x) \) are the strain rate and vorticity fields around the inclusion, that vary with position vector \( x \). \( E \) and \( W \) are the far-field strain rate and vorticity fields in the embedding medium. \( C^{\text{in}} \) and \( C \) are the 4\textsuperscript{th} order viscous stiffness tensors of the inclusion and the embedding medium respectively. Local fields (strain rate \( \varepsilon \), \( \varepsilon(x) \), and vorticity \( w \), \( w(x) \)) are related to respective far-field values (\( E \) and \( W \)) by partitioning equations, where \( A \) is the strain rate partitioning tensor, \( S \) and \( \Pi \) are respectively the 4\textsuperscript{th}-order symmetric and anti-symmetric Eshelby tensors (Jiang, 2014).
As expected from Eshelby’s solution, the velocity gradient fields inside an inclusion are constant, while the velocity gradient fields outside the inclusion vary with the position vector. To simulate a flanking structure, which is merely a deflection of planar or linear marker elements surrounding the inclusion, one needs to obtain velocity fields at every time step of calculation of the rotating and deforming inclusion (e.g., Jiang, 2007) and then use it to evaluate the displacements of linear or planar marker elements at that step.

The velocity gradient tensor $\mathbf{L}$ can be written as $L_{ij} = \frac{\partial v_i}{\partial x_j}$, which can be rearranged to determine the velocity field as:

$$\int_{x^o}^{x} dv_i = \int_{x^o}^{x} L_{ij} dx_j$$

where $v_i^o$ is the known velocity field at position vector $x^o$ which has coordinates $(x^o, y^o, z^o)$ and $v_i$ is the velocity field to be calculated at position vector $x$ which has coordinates $(x, y, z)$. $v_i$ and $v_i^o$ are the $i$th component of velocity vectors $\mathbf{v}$ and $\mathbf{v}^o$ respectively. Assuming the center of the inclusion to be at rest and since $\mathbf{L}$ is constant inside the inclusion, one can obtain the velocity field inside and at the inclusion surface as $v = \mathbf{L}x$, where $x$ is the position vector of the point defined in inclusion’s coordinate system. For any point outside the inclusion, velocity field can be evaluated as:

$$v_i = v_i^o + \int_{x^o}^{x} L_{ij} dx_j$$

(5.2)

where $x^o$ and $v^o$ are the known position and velocity vectors respectively at any point on inclusion’s surface. The problem now boils down to evaluating the integral in Eq.5.2 which can be discretized in the interval $(x^o, x)$. Eq. 5.2 can then be rewritten as follows:

$$v_i = v_i^o + \sum_{j=1}^{n} L_{ij}(x_j) \Delta x$$

(5.3)

Where, $n$ is the number of steps in which the interval $(x^o, x)$ is divided. $\Delta x$ is the interval of each step and $L_{ij}(x_j)$ is the velocity gradients evaluated at exterior points $x_j$ (Note that repeated indices imply summation). Exterior Eshelby solutions for inclusion
embedded in an isotropic medium are quick solutions with quasi-analytical accuracy (Jiang, 2016), therefore velocity gradient fields for all the exterior points can be quickly evaluated with high accuracy and efficiency.

In this investigation, we consider plane-strain general shearing flows as the far-field flow to understand the formation of flanking structures around cutting element of varying rheological contrast with the medium, initial shape, and orientation, deformed up to high finite strains. Our method here, however, also applies to any 3D general shearing flows (e.g., Jiang and Williams, 1998). In the coordinate system used in this investigation (Fig. 5.3), a general plane-strain general shearing flow is defined by the following Eulerian velocity gradient tensor:

\[
L = \begin{pmatrix}
\varepsilon & \gamma & 0 \\
0 & -\varepsilon & 0 \\
0 & 0 & 0 \\
\end{pmatrix}
\]

(5.4)

where \(\gamma (\gamma > 0)\) is the shear strain rate for the simple shearing component and \(\varepsilon (\varepsilon > 0)\) is the strain rate parallel to the X-axis. The flow in Eq.5.4 corresponds to a kinematic vorticity number \(W_k = \frac{\dot{\gamma}}{\sqrt{4\dot{\varepsilon}^2 + \dot{\gamma}^2}}\) (Jiang and White, 1995; Li and Jiang, 2011; Truesdell, 1953). We consider the variation of the flow by varying \(W_k\) from 0 to 1.

The cutting element’s initial shape is given by its three semi-axes: \(a_1 \geq a_2 \geq a_3\). To cover the shape variation of cutting element, we considered three reference initial shapes: prolate (10:1:1), oblate (10:10:1), sphere (1:1:1), and initial triaxial cutting elements with long and short semi-axial length fixed to 10 and 1 respectively and intermediate semi-axial length ranging from 2-9. These initial cutting elements will deform into various possible triaxial shapes in nature. The initial orientations of the cutting elements are defined by spherical angles (Jiang, 2007a, b). We consider two situations. In the first (Fig. 5.3a), we let \(a_1\) is aligned parallel to the Z-axis, and the initial orientation of the
cutting element is given by angle $\theta$, between $a_2$ axis and the X coordinate axis. For infinitely high values of $a_1$, this case is equivalent to the 2-D elliptical inclusion approaches (e.g., Mulchrone 2007). In the second case (Fig. 5.3b), we let the cutting element orient such that $a_1$ is oblique to the shear direction. This case considers the situation of cutting elements as in Exner and Dabrowski (2010).

![Diagram](image)

**Figure 5.3.** Geometry of the cutting element and the far field general plane straining flow. (a) Case where longest axis $a_1$ is normal to shearing direction, and the initial orientation of the cutting element is given by angle $\theta$. (b) Case where $a_1$ is oblique to the shear direction and the initial orientation is given by spherical angles ($\theta_1, \Phi_1, \theta_2$) for general triaxial cutting elements or ($\theta, \Phi$) for spheroidal cutting elements.

To measure the progression of the finite strain in plane strain general flows, we use strain intensity defined as $\rho = \sqrt{\left(\ln \frac{s_1}{s_2}\right)^2 + \left(\ln \frac{s_2}{s_3}\right)^2}$ where $s_1, s_2, s_3$ are the three principal stretches ($s_1 > s_2 > s_3$) of the finite strain ellipsoid (e.g., Yang et al., 2019). In the event
of simple shearing \((W_k = 1)\), the strain can also be measured by the shear strain \(\gamma\). The relation between \(\gamma\) and \(\rho\) in the simple shearing situation is shown in Fig. 5.4.

Since we wish to investigate how the variation in rheological contrast influences the formation of flanking structures, we consider the situations where the cutting element and the embedding medium are isotropic. The rheological contrast between the cutting element and the embedding medium is reduced to an effective viscosity ratio \(r\) between the cutting element to the embedding medium. Because of power-law rheology, \(r\) varies with time. We thus consider a range of constant \(r\) values. Grasemann et al. (2001) already showed the flanking structures developed for extremely strong \((r = 100)\) and extremely weak \((r = .01)\) cutting elements. We consider the values of \(r\) in the ranging between these two extremes.

\[ \text{Figure 5.4: The macroscale finite strain of the shear zone, measured by the strain intensity } \rho, \text{ as a function of shear strain } \gamma \text{ in simple shear case } (W_k = 1). \]

### 5.3 Modeling results

Fig. 5.5 present the 3-D flanking structures developed around cutting elements that are rheologically weaker \((r = .1, \text{ Fig. 5.5a})\) as well as stronger \((r=10, \text{ Fig. 5.5b})\) than the embedding medium, with an aspect ratio \((10:5:1)\) and initial orientation given by \(\theta = 135^\circ\)
and deformed under a macroscale simple shearing flow up to a shear strain of $\gamma = 2.5$. In Fig. 5.5a, the offset along the cutting element is antithetic to the shear sense and the deflection of the marker is concave towards the shear direction. The flanking structure can be regarded as a reverse a-type. In Fig. 5.5b, the offset along the cutting element is synthetic to the shear sense and the drag is convex towards the shear direction. The flanking structure can be regarded as normal s-type. Note that the term ‘normal’/‘reverse’ in flanking structure terminology (e.g., Grasemann et al. 2001) refers to the convex/concave deflection of the marker line in the shear direction along the cutting element respectively.

Figure 5.5: 3-D flanking structures developed around the cutting elements, that are rheologically weaker ($r = 0.1$, a, c) and rheologically stronger ($r = 10$, b, d) than the embedding medium, deformed up to shear strain $\gamma = 2.5$. The aspect ratio of the cutting element is 10:5:1, and the macroscale flow is dextral simple shearing ($W_x = 1$). (c) and (d) are 2-D cross-section view of (a) and (b) respectively.
Figs. 5.6 presents the 2-D cross-sections (along the X-Y plane) of flanking structures developed around cutting elements that are rheologically stronger \((r = 10)\) as well as weaker \((r = 0.1)\) than the embedding medium, with sectional aspect ratio 5:1, and different

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<td>(r = 0.1, \gamma = 5)</td>
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<td>(r = 10, \gamma = 2.5)</td>
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Figure 5.6: 2-D cross sections (along the X-Y plane) of the flanking structures developed around the cutting elements, that are rheologically weaker \((r = 0.1, a-f)\) and rheologically stronger \((r = 10, g-l)\) than the embedding medium, deformed up to shear strain \(\gamma = 5\). The sectional aspect ratio of the cutting element is 5:1, and the macroscale flow is simple shearing \((W_k = 1)\).
initial orientations given by $\theta$ and deformed under a macroscale flow with $W = 1$, up to finite strain $\rho = 5$. Depending on initial orientations and rheological contrast of the cutting element to the embedding medium, various types (namely normal or reverse s-, n- and a-type) flanking structures can be formed as labeled in the figures. Simulation results for more general plane strain flows with $W < 1$ are available in the online repository (link provided in Appendix G).

Fig. 5.7 shows the variation in flanking structures with respect to $r$. Note that as $r$ approaches unity, the radius of curvature of the flanking structure reduces and the flanking structures are almost planar. This can even change the drag from convex up to concave up as in Fig. 5.7 g-i. For cutting elements with $r < 1$, as the $r$ goes to unity, the a-type flanking structure does not transition to an s-type flanking structure at a high finite strain of $\gamma = 5$ (Fig. 5.7 b, c).

Fig. 5.8 shows the variation in flanking structures for different sectional aspect ratios. We note that the aspect ratios do not affect the overall shape of the flanking structures at low finite strains ($\gamma = 2.5$), however, at higher finite strains ($\gamma = 5$), the flanking structures may be different. For example, for lower aspect ratio 3:1, the a-type flanking structure (Fig. 5.8a) may transition to an s-type (Fig. 5.8c) in case of weak cutting elements ($r = 0.1$). This does not happen for aspect ratio 8:1 (Figs. 5.8b, d).

Fig. 5.9 shows the 3-D flanking structures where the cutting element is oblique to the shear direction with the orientation given by spherical angles ($0^\circ$, $30^\circ$, $135^\circ$). This causes the linear elements to deflect both vertically as well as laterally along the cutting element (Figs. 5.9b, d). Our result for a rheologically weak cutting element with $r = 0.1$ is similar to that of Exner and Dabrowski (2010) who simulated flanking structures around an inviscid cutting element. For a stronger cutting element with $r = 10$, we found that the lateral offset can be in the opposite sense as compared to $r = 0.1$ (Fig. 5.9 c, e).

Additional simulation results and video animations of the flanking structures can be accessed from the online GitHub repository (link provided in Appendix G).
Figure 5.7: Variation in flanking structures as a function of $r$. The figure presents 2-D cross sections (along the X-Y plane) of the flanking structures around cutting elements with $r < 1$ (a-f) and $r > 1$ (g-l), deformed up to shear strain $\gamma = 5$. The initial orientation is given by $\theta=120^\circ$, the sectional aspect ratio of the cutting element is 5:1, and the macroscale flow is simple shearing.
Figure 5.8: Variation in flanking structures with sectional aspect ratio of the cutting element. The figure presents 2-D cross sections (along the X-Y plane) of the flanking structures around cutting elements with $r=0.1$, deformed up to shear strain $\gamma = 5$. The initial orientation is given by $\theta=120^\circ$ and the macroscale flow is simple shearing.
Figure 5.9: 3-D flanking structures developed around the cutting elements oblique to the shear direction with orientation given by spherical angles \((0^\circ, 30^\circ, 135^\circ)\) for \(r = 10\) (b, c) and \(r = 0.1\) (d, e) deformed up to shear strain \(\gamma = 2.5\). The initial aspect ratio of the cutting element is 10:5:1, and the macroscale flow is dextral simple shearing \((W_L=1)\) (a) initial configuration of the cutting element and linear markers in X-Z plane (b) and (d) are 3-D views of deformed linear markers, whereas (c) and (e) are the top-view (along X-Z plane) showing the lateral offset along the cutting element.
5.4 A reverse dynamic modeling approach to extract kinematic information from shear zones

In the previous section, we demonstrated how a flanking structure can be influenced by the variation of the cutting element’s viscosity, its aspect ratios, initial orientation, and flow type. In this section, we develop a reverse dynamic modeling approach, following Kocher and Mancktelow (2005), to quantitatively estimate the kinematic information from the observed flanking structures in the natural ductile shear zones. Since there is limited information regarding the 3-D geometry of the cutting element, we assume the cutting element to be cylindrical, with its longest axes infinitely long. The approach can be briefly described as follows (Fig. 5.10a): If the shear sense of the bulk flow is known from independent evidence, one can digitize the given flanking structure from the photograph and reverse deform it for a range of initial parameters given by reverse kinematic vorticity $W_k$, number of calculation time steps $t$, and viscosity ratio $r$ of the cutting element to the embedding medium. The parameters $W_k$, $t$, and $r$ for which the digitized markers are close to the initial assumed configuration are the parameters corresponding to which the flanking structures were formed. Note that Kocher and Mancktelow (2005) followed a similar approach, however, they assume the cutting element to have infinitely low viscosity. Our approach generalizes their work and can be applied to cutting elements with more variable viscosities.

The amount of how close the markers are from the initial configuration can be quantified using the residual $R$ at time $t$ (K Kocher and Mancktelow, 2005) given by:

$$R_t = \sum_{j=1}^{nlines} \frac{1}{npts_j} \sum_{i=1}^{npts_j} \sqrt{(y(t)-y_{mean})^2},$$

where $j$ is the index of the marker line that is digitized, $y_{mean}$ is the mean $y$-position of the line $j$ at time $t$, $i$ is the index of the point on respective line $j$, $npts_j$ is the number of points in line $j$, and $nlines$ are the total number of digitized marker lines. To compare the fit of a marker geometry at time $t$ to the initial configuration, the residual can be defined as $R = R_t / R_0$, where $R_0$ is the residual of the structure at the time $t = 0$. 152
Figure 5.10: Reverse dynamic modelling approach to quantitatively estimate kinematic information (a) illustration of the approach (b)-(c) Natural flanking structures on which the approach is applied. (b) Flanking structure in alternating mylonitic calcite and dolomitic layers (darker) from Naxos, Greece (Modified after Kocher and Mancktelow 2005) (c) Flanking microstructure with quartz veins (white ellipse) as the cutting element and compositional layering as host elements, from Cross Lake greenstone belt, Manitoba, Canada. Red dots indicate digitization of the markers.
\( \mathbf{R} \) is a function of \( W_k, t \) and \( r \). The problem then becomes finding the global minimum of \( \mathbf{R} \). The parameters for which \( \mathbf{R} \) is minimized will correspond to the parameters for which the flanking structures were formed. We present two geological examples on which this reverse modeling is applied, and quantitative kinematic information has been estimated. Fig. 5.10b shows a flanking structure in alternating mylonitic calcite and dolomitic layers (darker) from Naxos, Greece (Kocher and Mancktelow 2005). The shape of the cutting element is approximated by an elongated ellipse (Fig. 5.10b). Our reverse modelling estimates the \( W_k = 0.95 \), \( r \sim 0.05 \), and strain intensity \( \rho = 0.88 \), which can be evaluated from \( W_k \) and \( t \). Our results for this flanking structure compare well with the model of Mancktelow and Kocher (2005), who estimated a \( W_k = 0.95 \) while assuming \( r = 10^{-12} \).

Fig. 5.10c shows a flanking structure around a quartz vein as the cutting element surrounded by compositional layering as host elements, from Cross lake greenstone belt, Manitoba, Canada. The shape of such quartz vein is approximated by a closely fitted ellipse (Fig. 5.10c). Our reverse modelling estimates the \( W_k = 1 \), \( r \sim 15 \), and \( \rho = 1.9 \). The value of \( r > 1 \) and \( W_k = 1 \) is consistent with the flanking structures simulated in this work as well as previous models (e.g., Grasemann et al., 2001), specifically the flanking folds, around the cutting element, and implies that quartz veins behaved as the stronger heterogeneous element than the embedding medium subjected to a simple shear dominated flow. The \( \rho \) gives the estimate of finite strain accumulated since the formation of the quartz veins.

Note that in the above calculations, strain intensity is used as a proxy for time, since the actual strain rates in deformed rocks are not known a priori. If strain rate estimates are known from independent evidence, one can use the strain intensity information to estimate the time taken to form the structure.
5.5 Discussion and Conclusions

We have simulated 3-D flanking structures around a cutting element with varying rheological contrast with the ambient medium, initial shape, and orientation and deformed up to high finite strains ($\gamma=5$). Our models reproduce the different types of flanking structures namely, a-type, n-type, and s-type flanking structures around cutting elements. In contrast to the previous models with limited cutting element geometry and rheological properties (e.g., Grasemann et al., 2001), our modeling results show that all three types of flanking structures can be formed around any cutting element stronger ($r=10$) than the embedding medium. We have demonstrated the variation in flanking structures depending on the initial aspect ratio of the cutting element, viscosity ratio, orientation as well as macroscale finite strain.

Our numerical simulations correlate well with the analogue experiments of Exner et al. (2004) who found that the flanking structure around a weak inviscid cutting element may transition from an a-type to s-type flanking structure at high finite strains. However, we note that this transition depends on the cutting element’s viscosity and macroscale finite strain. Our models of 3-D flanking structures displaying lateral offsets can be compared to Exner and Dabrowski (2010) who simulated the cutting element as an elliptical crack filled with inviscid material. Our modeling results of $r > 1$ show how the lateral offset may vary with the viscosity ratio, which might not always be inviscid. In all, our work demonstrates that variations in viscosities of the cutting elements may produce varying flanking structures and care must be taken while studying a natural flanking structure since the rheology of any cutting element is not known apriori.

We have developed a reverse-dynamic modeling tool that can provide a quantitative estimate of flow vorticity, finite strain, and cutting element’s viscosity relative to the embedding medium from an observed natural flanking structure. This model generalizes the work of Kocher and Mancktelow (2005) who performed a similar analysis but assumed the cutting element as an inviscid material. We have applied this reverse dynamic model and determined flow vorticity, finite strain, and cutting element’s viscosity relative to the embedding medium for some natural examples of flanking
structures from ductile shear zones. This approach (MATLAB code link in Appendix G) serves as a toolbox for any structural geologist to determine kinematic information from ductile shear zones and provide quantitative kinematic information on regional tectonics.

5.6 References


Jiang, D., 2007a. Numerical modeling of the motion of rigid ellipsoidal objects in slow


Wiesmayr, G., Grasemann, B., 2005. Sense and non-sense of shear in flanking structures

Chapter 6

6 Conclusions and future work

6.1 Conclusions

This thesis has made contributions to the understanding of how the heterogeneous rheology of Earth’s lithosphere influence various kinds of geological rock records such as mineral assemblages, quartz c-axis fabrics, and flanking structures.

The main contributions are summarized below:

(1) MOPLA has been applied to the long-standing problem of tectonic pressure deviation in Earth’s lithosphere. We found that the pressure deviations due to tectonic deformation are in the order of deviatoric stresses and hence limited by the strength of rocks. While the short-term elastic interactions may cause high deviatoric stresses, and hence high-pressure deviations, for long-term geological timescales of ~Myr, such pressure deviations are irrelevant compared to the lithostatic pressure values. This work supports the usage of conventional geothermobarometry-based pressure estimates as a proxy for depth in geodynamic models.

(2) A multiscale approach coupling MOPLA and VPSC is used to simulate quartz c-axis fabrics in heterogeneous shear zones. It has been found that the well-known quartz c-axis fabric variation, showing apparent opposite senses of shear within a single thin section, is due to partitioned flow within the quartz domains and reflects a finite strain gradient rather than a reversal of vorticity sense as previously thought. While the flow vorticity within the rheologically heterogeneous quartz domains may vary from the bulk vorticity, the sense of the vorticity always remains the same. Because of flow partitioning, it is not possible to estimate the vorticity number of the macroscale flow from quartz c-axis fabrics. But it is still possible to obtain the macroscale vorticity axis by averaging the
microscale vorticity axes from quartz RDEs. The latter can be obtained through the c-axis vorticity axis analysis.

(3) 3-D flanking structures are simulated using a new approach developed in this thesis. It has been demonstrated how flanking structure may vary with rheological contrast of the cutting element to the embedding medium, the 3-D aspect ratio of the cutting element, 3-D flow, and orientation of the cutting element. A reverse-dynamic modeling approach is then developed and applied to quantitatively estimate useful information such as cutting element’s viscosity, finite strains, and kinematic vorticity of the flow from observed natural flanking structures. This reverse-dynamic model serves as a useful toolbox for any structural geologist aiming to estimate kinematic information on any regional tectonic setting with flanking structure outcrops (MATLAB code link provided in Appendix G).

(4) This thesis developed a new algorithm using MATLAB vectorization to evaluate mechanical fields around a viscous inclusion embedded in a general anisotropic viscous medium. These solutions have wide applications in simulating the heterogeneous deformation of anisotropic rocks. The open-source MATLAB code is available from the online GitHub repository link provided in Appendix A.

(5) A MATLAB implementation has been developed coupling MOPLA with the VPSC model to capture the influence of flow partitioning on the c-axis fabrics. The MATLAB code is available from the online GitHub repository link in Appendix B.

(6) A new approach along with MATLAB implementation for simulating flanking structures has been developed that allows the incorporation of parameters such as variable rheological contrast of the cutting element to the embedding medium, the 3-D aspect ratio of the cutting element, 3-D flow, and orientation of the cutting element. This model has wide application for simulating flanking structures in natural shear zones. The open-source MATLAB code is available from the online GitHub repository link provided in Appendix E.
6.2 Future work

Understanding the dynamics of planet Earth through numerical models is the broad objective of my research. In this thesis, mainly viscous rheology of rocks has been considered to capture the geodynamic processes occurring at the geological timescales of \sim\text{Myr}. For my future research, my goal is to incorporate more complex rheologies in numerical models applicable at the short-term timescales (\sim100-1000 yrs.) such as viscoelastic rheology as well as rate-and state-friction. The broad question that my future research will try to answer is how the long-term tectonic deformation processes couples with the short-term geodynamic processes such as earthquakes, slow-slip events and how it may influence various geological rock records (e.g., Jamveit et al., 2019).

While this thesis has effectively demonstrated how the rheological heterogeneities in Earth’s lithosphere influence the formation of geological rock records, several open questions remain that I plan to work on in the recent future. Some of them are summarized as follows:

The flanking structure model developed in this work assumes the embedding medium as an isotropic system and applies to cases where the rheological anisotropy is insignificant. Although the formulation used in this work theoretically allows the system to be general anisotropic, due to the complexity of the mathematical formulation, the current MATLAB-based code cannot be efficiently used for a large number of velocity field calculations in an anisotropic medium. Thus, future efforts will be made in further optimizing the code by transferring the numerical model to a faster computing language such as Julia or C++. A more efficient computation can even allow the anisotropic formulations to be used in a reverse dynamic modeling approach as in this thesis, to further get some quantitative estimates of rheological anisotropy in rocks.

While this thesis work clearly illustrates the influence of flow partitioning on quartz c-axis fabrics, the specific details of how secondary phases such as mica or feldspar (their volume fraction and c-axis fabric) may influence quartz c-axis fabrics in mylonites are not clear. Despite the wide occurrence of quartz aggregates surrounded by secondary phases in natural mylonites, only a few investigations have studied such phenomenon
(e.g., Cross et al., 2017). The VPSC model can allow the simulation of c-axis fabrics with multiple phases of mineral assemblages. Thus, understanding the effects of secondary mineral phases such as feldspar and mica on quartz c-axis fabrics in natural mylonites will form another aspect of my future research.

As evident in this thesis, rheological heterogeneity in Earth’s lithosphere strongly governs the dynamics of rocks and hence needs to be considered in future numerical models of geodynamic processes. A specific example is that of slow-earthquakes occurring at the brittle-ductile transition zone of Earth’s lithosphere. Geological examples of slow-earthquakes (e.g., Behr et al., 2018) clearly show fault slips within the rheologically heterogeneous eclogite units embedded in a matrix undergoing ductile deformation. However, none of the available slow-earthquake models (e.g., Liu and Rice, 2007.) consider such complex rheologies. To consider such variations in rock rheology, more sophisticated numerical models such as Pylith based finite element models (e.g., Aagaard et al., 2013) coupling visco-elastic rheology with rate-and-state fault friction are required. Understanding the physics of slow earthquakes by considering the influence of partitioned flow on the slow-fault slip will form another aspect of my future research.
6.3 References


Appendices

Appendix A. Link and Description of MATLAB code for Exterior Eshelby solution in general anisotropic medium

There are two versions of MATLAB functions for evaluating auxiliary tensors $\Lambda^E(x)$ and $T^E(x)$: first, the non-vectorized version, and second, the vectorized version. Brief description of each function file are given as follows:

Non-vectorized functions:

$\text{LambdaExtAniso3DPress_nv.m}$: is to calculate auxiliary tensor for pressure $\Lambda^E(x)$ for an exterior point around an inclusion embedded in an anisotropic viscous medium. Its inputs are vector $a_i$ corresponding to semi-axial lengths of the ellipsoidal inclusion, a vector $x_i$ corresponding to three coordinates of an exterior point, a fourth-order stiffness tensor of the embedding medium $C_{ijkl}$ represented by a $3\times3\times3\times3$ matrix, $1\times N$ matrices corresponding to Gaussian grid nodes $\Theta_\rho$ and $\Phi_\varphi$, $1\times N$ matrix corresponding to Gaussian weights $w_\rho$, $1\times n_\psi$ matrix corresponding to Gaussian grid nodes $\Psi_\varphi$ and $1\times n_\psi$ matrix corresponding to Gaussian weights $w_\psi$. $N$ is the total number of grid nodes in product Gaussian quadrature corresponding to $(\Theta_\rho, \Phi_\varphi)$ and $n_\psi$ is the number of nodes for Gaussian quadrature corresponding to $\Psi_\varphi$.

$\text{AuxTensorPressOutAniso_nv.m}$: is to calculate each element of the auxiliary tensor for pressure $\Lambda^E(x)$. Its inputs are: vector $\text{sub}_j$ corresponding to two indices of the auxiliary tensor, vector $a_i$ corresponding to semi-axial lengths of the ellipsoidal inclusion, a vector $x_i$ corresponding to three coordinates of an exterior point, a fourth-order stiffness tensor of the embedding medium $C_{ijkl}$, $1\times N$ matrices corresponding to Gaussian grid nodes $\Theta_\rho$
and $\phi_q$, $1 \times N$ matrix corresponding to Gaussian weights $W_p$, $1 \times n_\nu$ matrix corresponding to Gaussian grid nodes $\psi_j$ and $1 \times n_\nu$ matrix corresponding to Gaussian weights $W_j$.

**DP.m**: is to evaluate the integrand $\frac{H_i(x-x')\tilde{\xi}_j}{a_j}$ described in the text. Its inputs are:

- vector $a_i$ corresponding to semi-axial lengths of the ellipsoidal inclusion,
- vector $x_i$ corresponding to three coordinates of an exterior point,
- a fourth-order stiffness tensor of the embedding medium $C_{ijkl}$,
- $1 \times N$ matrices corresponding to Gaussian grid nodes $\theta_p$ and $\phi_q$,
- $1 \times n_\nu$ matrix corresponding to Gaussian grid nodes $\psi_j$ and $1 \times n_\nu$ matrix corresponding to Gaussian weights $W_j$.

**Hm.m**: is to evaluate Green’s function for pressure $H_i(x)$ described in the text. Its inputs are:

- vector $x_i$ corresponding to three coordinates of an exterior point and a fourth-order stiffness tensor of the embedding medium $C_{ijkl}$.

**ZZone.m**: is to evaluate the terms $z, (z_p\hat{x}_q + z_q\hat{x}_p)$, and $\hat{x}_i = \frac{x_i}{r}$ described in the text. Its inputs are:

- vector $x_i$ corresponding to three coordinates of an exterior point and a $1 \times n_\nu$ matrix corresponding to Gaussian grid nodes $\psi_j$.

**Akm.m**: is to evaluate the terms $\hat{A}, \xi$, and $\lambda$ by performing $\left(\begin{array}{cc} \hat{A} & \xi \\ \xi^T & \lambda \end{array}\right) = \left(\begin{array}{cc} A & z \\ z^T & 0 \end{array}\right)^{-1}$. Its inputs are:

- a fourth-order stiffness tensor of the embedding medium $C_{ijkl}$,
- a $3 \times n_\nu$ matrix corresponding to $z$ evaluated for Gaussian grid nodes $\psi_j$.
**MultimixM.m**: performs a mixing operation corresponding to \( C_{ap\beta\gamma}(z_p \hat{x}_q + z_q \hat{x}_p) \). Its inputs are: a fourth-order stiffness tensor of the embedding medium \( C_{ijkl} \), a \( 3 \times 3 \times n_\nu \) matrix corresponding to \( (z_p \hat{x}_q + z_q \hat{x}_p) \) evaluated for Gaussian grid nodes \( \psi_j \).

**T_ExtAniso3D.m**: is to calculate Green’s tensor \( T^E(x) \) for an exterior point around an inclusion embedded in an anisotropic viscous medium. Its inputs are: vector \( a_i \) corresponding to semi-axial lengths of the ellipsoidal inclusion, a vector \( x_i \) corresponding to three coordinates of an exterior point, a fourth-order stiffness tensor of the embedding medium \( C_{ijkl} \), \( 1 \times N \) matrix corresponding to Gaussian grid nodes \( (\theta_{\rho}, \phi_q) \), \( 1 \times N \) matrix corresponding to Gaussian weights \( w_{\rho} \), \( 1 \times n_\nu \) matrix corresponding to Gaussian grid nodes \( \psi_j \) and \( 1 \times n_\nu \) matrix corresponding to Gaussian weights \( w_j \).

**GreenTensorOutAniso.m**: is to calculate each element of the Green’s tensor \( T^E(x) \). Its inputs are: vector \( sub_i \) corresponding to 4 indices of the Green’s tensor, a vector \( a_i \) corresponding to semi-axial lengths of the ellipsoidal inclusion, a vector \( x_i \) corresponding to three coordinates of an exterior point, a fourth-order stiffness tensor of the embedding medium \( C_{ijkl} \), \( 1 \times N \) matrices corresponding to Gaussian grid nodes \( \theta_{\rho} \) and \( \phi_q \), \( 1 \times N \) matrix corresponding to Gaussian weights \( w_{\rho} \), \( 1 \times n_\nu \) matrix corresponding to Gaussian grid nodes \( \psi_j \) and \( 1 \times n_\nu \) matrix corresponding to Gaussian weights \( w_j \).

**DT.m**: is to evaluate the integrand \( \frac{G_{ikjli}(x-x')\xi_j}{a_j} \) described in the text. Its inputs are: vector \( a_i \) corresponding to semi-axial lengths of the ellipsoidal inclusion, a vector \( x_i \) corresponding to three coordinates of an exterior point, a fourth-order stiffness tensor of the embedding medium \( C_{ijkl} \), \( 1 \times N \) matrices corresponding to Gaussian grid nodes \( \theta_{\rho} \) and
\( \phi_q, 1 \times n_q \) matrix corresponding to Gaussian grid nodes \( \psi_j \) and \( 1 \times n_q \) matrix corresponding to Gaussian weights \( w_j \).

**Gm.m:** is to evaluate the derivative of Green’s function for velocity \( G_{ik,l}(x-x') \) described in the text. Its inputs are: vector \( x_i \) corresponding to three coordinates of an exterior point, and a fourth-order stiffness tensor of the embedding medium \( C_{ijkl}, 1 \times n_q \) matrix corresponding to Gaussian grid nodes \( \psi_j \), and \( 1 \times n_q \) matrix corresponding to Gaussian weights \( w_j \).

**Vectorized functions:**

*LambdaExtAniso3DPress_vec.m:* is to calculate auxiliary tensor for pressure \( \Lambda^E(x) \) for an exterior point around an inclusion embedded in an anisotropic viscous medium. Its inputs are: vector \( a_i \) corresponding to semi-axial lengths of the ellipsoidal inclusion, a vector \( x_i \) corresponding to three coordinates of an exterior point, a fourth-order stiffness tensor of the embedding medium \( C_{ijkl}, 1 \times N \) matrices corresponding to Gaussian grid nodes \( \theta_p \) and \( \phi_q \), \( 1 \times N \) matrix corresponding to Gaussian weights \( w_p \), \( 1 \times n_q \) matrix corresponding to Gaussian grid nodes \( \psi_j \) and \( 1 \times n_q \) matrix corresponding to Gaussian weights \( w_j \). \( N \) is the total number of grid nodes in product Gaussian quadrature corresponding to \( (\theta_p, \phi_q) \) and \( n_q \) is the number of nodes for Gaussian quadrature corresponding to \( \psi_j \).

*AuxTensorPressOut_vec.m:* is to calculate each element of the auxiliary tensor for pressure \( \Lambda^E(x) \). Its inputs are: vector \( sub_i \) corresponding to two indices of the auxiliary tensor, vector \( a_i \) corresponding to semi-axial lengths of the ellipsoidal inclusion, a vector
\( x_i \) corresponding to three coordinates of an exterior point, a fourth-order stiffness tensor of the embedding medium \( C_{ijkl} \), 1×\( N \) matrices corresponding to Gaussian grid nodes \( \Theta_p \) and \( \phi_q \), 1×\( N \) matrix corresponding to Gaussian weights \( \Psi_p \), 1×\( n_{\psi} \) matrix corresponding to Gaussian grid nodes \( \psi_f \) and 1×\( n_{\psi} \) matrix corresponding to Gaussian weights \( w_j \).

**DP_vec.m:** is to evaluate the integrand \( \frac{H_i(x-x')\hat{z}_j}{a_j} \) described in the text. Its inputs are: vector \( a_i \) corresponding to semi-axial lengths of the ellipsoidal inclusion, a vector \( x_i \) corresponding to three coordinates of an exterior point, a fourth-order stiffness tensor of the embedding medium \( C_{ijkl} \), 1×\( N \) matrices corresponding to Gaussian grid nodes \( \Theta_p \) and \( \phi_q \), 1×\( n_{\psi} \) matrix corresponding to Gaussian grid nodes \( \psi_f \) and 1×\( n_{\psi} \) matrix corresponding to Gaussian weights \( w_j \).

**Hm_vec.m:** is to evaluate Green’s function for pressure \( H_i(x-x') \) described in the text. Note that this function evaluates a vectorized version where \( H_i(x-x') \) is a 1×\( N \) matrix. Its inputs are: a 3×\( N \) matrix \( X \) corresponding to \( (x-x') \) evaluated for \( N \) grid nodes, a fourth-order stiffness tensor of the embedding medium \( C_{ijkl} \), 1×\( n_{\psi} \) matrix corresponding to Gaussian grid nodes \( \psi_f \), and 1×\( n_{\psi} \) matrix corresponding to Gaussian weights \( w_j \).

**ZZ_vec.m:** is to evaluate the terms \( z_i, (z_p\hat{x}_q + z_q\hat{x}_p) \), and \( \hat{x}_i = \frac{x_i}{r} \) described in the text. Its inputs are: a 3×\( N \) matrix \( X \) corresponding to \( (x-x') \) evaluated for \( N \) grid nodes and a 1×\( n_{\psi} \) matrix corresponding to Gaussian grid nodes \( \psi_f \).
**Akmm_vec.m:** is to evaluate the terms $\vec{A}, \zeta,$ and $\hat{\lambda}$ by performing
\[
\begin{pmatrix}
\vec{A} & \zeta \\
\zeta^T & \hat{\lambda}
\end{pmatrix} ^{-1} = \begin{pmatrix} A & z \\ z^T & 0 \end{pmatrix}^{-1}.
\] Its inputs are: a fourth-order stiffness tensor of the embedding medium $C_{ijkl}$, a $3 \times N \times n_{\psi}$ matrix corresponding to $z$ evaluated for Gaussian grid nodes $(\theta_p, \phi_q)$ and $\psi_j$.

**MultimixMMvec.m:** performs a mixing operation corresponding to
\[
C_{\alpha\beta\gamma\delta}(z_p \hat{x}_q + z_q \hat{x}_p).
\] Its inputs are: a fourth-order stiffness tensor of the embedding medium $C_{ijkl}$, a $3 \times 3 \times N \times n_{\psi}$ matrix corresponding to $(z_p \hat{x}_q + z_q \hat{x}_p)$ evaluated for Gaussian grid nodes $(\theta_p, \phi_q)$ and $\psi_j$.

**T_ExtAniso3D_vec.m:** is to calculate Green’s tensor $T^E(x)$ for an exterior point around an inclusion embedded in an anisotropic viscous medium. Its inputs are: vector $a_i$ corresponding to semi-axial lengths of the ellipsoidal inclusion, a vector $x_i$ corresponding to three coordinates of an exterior point, a fourth-order stiffness tensor of the embedding medium $C_{ijkl}$, $1 \times N$ matrix corresponding to Gaussian grid nodes $(\theta_p, \phi_q)$, $1 \times N$ matrix corresponding to Gaussian weights $w_p$, $1 \times n_{\psi}$ matrix corresponding to Gaussian grid nodes $\psi_j$ and $1 \times n_{\psi}$ matrix corresponding to Gaussian weights $w_j$.

**GreenTensorOutAniso_vec.m:** is to calculate each element of the Green’s tensor $T^E(x)$. Its inputs are: vector $s McCl$ corresponding to 4 indices of the Green’s tensor, a vector $a_i$ corresponding to semi-axial lengths of the ellipsoidal inclusion, a vector $x_i$ corresponding to three coordinates of an exterior point, a fourth-order stiffness tensor of the embedding medium $C_{ijkl}$, $1 \times N$ matrices corresponding to Gaussian grid nodes $\theta_p$ and $\phi_q$, $1 \times N$ matrix corresponding to Gaussian weights $w_p$, $1 \times n_{\psi}$ matrix corresponding to Gaussian grid nodes $\psi_j$ and $1 \times n_{\psi}$ matrix corresponding to Gaussian weights $w_j$.

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DT_vec.m: is to evaluate the integrand $\frac{G_{ik,l}(x-x')\xi_j}{a_j}$ described in the text. Its inputs are:

- vector $a_i$ corresponding to semi-axial lengths of the ellipsoidal inclusion,
- a vector $x_i$ corresponding to three coordinates of an exterior point,
- a fourth-order stiffness tensor of the embedding medium $C_{ijkl}$,
- $1 \times N$ matrices corresponding to Gaussian grid nodes $\theta_p$ and $\phi_q$, $1 \times n_\nu$ matrix corresponding to Gaussian grid nodes $\psi_j$, and $1 \times n_\nu$ matrix corresponding to Gaussian weights $w_j$.

Gm_vec.m: is to evaluate the derivative of Green’s function for velocity $G_{ik,l}(x-x')$ described in the text. Note that this function evaluates a vectorized version where $G_{ik,l}(x-x')$ is $1 \times N$ matrix. Its inputs are:

- a $3 \times N$ matrix $X$ corresponding to $(x-x')$ evaluated for $N$ grid nodes,
- a fourth-order stiffness tensor of the embedding medium $C_{ijkl}$,
- $1 \times n_\nu$ matrix corresponding to Gaussian grid nodes $\psi_j$, and $1 \times n_\nu$ matrix corresponding to Gaussian weights $w_j$.

Other MATLAB files:

The following MATLAB files use the above functions to evaluate exterior Eshelby fields:

- CompareLambda_code_vecVSnv.m: Compares the auxiliary tensor for pressure $\Lambda^E(x)$ calculated for some exterior points around inclusion for both vectorized and non-vectorized code.

- CompareT_code_vecVSnv.m: Compares the Green’s tensor $T^E(x)$ calculated for some exterior points around inclusion for both vectorized and non-vectorized code.

- ComparePress_code_isoVSaniso.m: Benchmark above code for anisotropic medium with known isotropic solutions with quasi-analytical accuracy. $\Lambda^E(x)$ evaluated for exterior
point around an inclusion using both solutions with quasi-analytical accuracy for isotropic medium and the code developed in this work.

*CompareStress_code_isoVSaniso.m:* Benchmark the above code for anisotropic medium with known isotropic solutions. $S^e(x)$ evaluated for exterior points around an inclusion using both isotropic solutions and the code developed in this work.

*PlotIsosurface3Dpress.m:* plots 3-D pressure fields as iso-surfaces around an inclusion embedded in a general anisotropic medium.

*Plot_Cross_section_Pressurefield.m:* plots X-Y and X-Z cross-sections of pressure fields around an inclusion embedded in a general anisotropic medium.

*PlotIsosurface3DStress.m:* plots 3-D stress fields (stress invariants) as iso-surfaces around an inclusion embedded in a general anisotropic medium.

*Plot_Cross_section_Stressfield.m:* plots X-Y and X-Z cross-sections of stress fields (stress invariants) around an inclusion embedded in a general anisotropic medium.

**Link for GitHub repository of the MATLAB code:**

https://github.com/ankibues/MOPLA_Application_Matlab/tree/master/PressureInvestigation/PressureCalc/ForAnisotropic%20case/3D%20case
Appendix B: Link for GitHub repository of the MATLAB implementation coupling VPSC and MOPLA

https://github.com/ankibues/MOPLA_Application_Matlab/tree/master/MOPLA_coupling_VPSC
Appendix C: Cartesian to Elliptic coordinates transformation and vice-versa

The Elliptical coordinate system \((\xi, \eta)\) is a two-dimensional orthogonal coordinate system comprised of confocal ellipses and hyperbolae (See Fig. 4.2b in the text). The transformation from Elliptic to Cartesian coordinate is given by:

\[
\begin{align*}
  x &= c \cosh(\xi) \cos(\eta) \\
  y &= c \sinh(\xi) \sin(\eta) \\
  c^2 &= a^2 - b^2 \\
  \xi &\geq 0 \quad , \quad 0 \leq \eta < 2\pi
\end{align*}
\]

Where \(a\) and \(b\) are the semi-major and semi-minor axes of the ellipse, and \(c\) is the elliptical eccentricity.

Sun (2017) derived the explicit expression for converting Cartesian coordinates to Elliptic coordinates. They are summarized as follows:

\[
\begin{align*}
  \eta &= \eta_0 \cdot x \geq 0, y \geq 0 \\
  \eta &= \pi - \eta_0 \cdot x < 0, y \geq 0 \\
  \eta &= \pi + \eta_0 \cdot x \leq 0, y < 0 \\
  \eta &= 2\pi - \eta_0 \cdot x > 0, y < 0 \\
  \xi &= \frac{1}{2} \ln(1 - 2q + 2\sqrt{q^2 - q})
\end{align*}
\]
Where $\eta_0 = \arcsin(p)$, $p = \frac{-B + \sqrt{B^2 + 4c^2y^2}}{2c^2}$, $q = \frac{-B - \sqrt{B^2 + 4c^2y^2}}{2c^2}$ and $B = x^2 + y^2 - c^2$.

**Appendix D: Cartesian to Ellipsoidal coordinates transformation and vice-versa**

The Cartesian coordinates $(X, Y, Z)$ can be calculated from the respective Ellipsoidal coordinates $(\varphi, \lambda, h)$ using the following relation:

$$X = (N + h) \cos \varphi \cos \lambda$$

$$Y = [N (1 - ee^2) + h] \cos \varphi \sin \lambda$$

$$Z = [N (1 - ex^2) + h] \sin \varphi$$

where $\varphi (-\pi/2 \leq \varphi \leq +\pi/2)$ is the latitude, $\lambda (-\pi < \lambda \leq +\pi)$ is the longitude, $h (-b \leq h < +\infty)$ is the (ellipsoidal) height (See Fig. 4.3b).

$$N = \frac{ax}{\sqrt{1 - ex^2 \sin^2 \varphi - ee^2 \cos^2 \varphi \sin^2 \lambda}}$$

is the radius of curvature in the prime vertical normal section, where

$$ex^2 = ax^2 - b^2/ax^2$$

and

$$ee^2 = ax^2 - ay^2/ax^2$$

are the first eccentricities squared of the triaxial ellipsoid.

The above calculations are straightforward. To obtain Ellipsoidal coordinates $(\varphi, \lambda, h)$ from the Cartesian coordinates $(X, Y, Z)$, one needs to obtain the projection $(x, y, z)$ of the point $(X, Y, Z)$ onto this ellipsoid along the normal to this surface, also known as the
foot point. This can be evaluated using the Bisection method as in Eberly (2018). Once \((x, y, z)\) is known, \(\varphi\) and \(\lambda\) can be evaluated as follows:

\[
\varphi = \arctan \left[ \frac{(1-ee^2)z}{(1-ex^2)(1-ee^2)x^2 + y^2} \right], \text{ if } (1-ee^2)z \leq (1-ex^2)\sqrt{(1-ee^2)x^2 + y^2}
\]

or

\[
\varphi = \frac{\pi}{2} - \arctan \left[ \frac{(1-ex^2)\sqrt{(1-ee^2)x^2 + y^2}}{(1-ee^2)z} \right], \text{ if } (1-ee^2)z > (1-ex^2)\sqrt{(1-ee^2)x^2 + y^2}
\]

The conventions with regard to the proper quadrant for \(\varphi\) are applied from the sign of \(Z\).

\[
\lambda = 2\arctan \left[ \frac{y}{(1-ee^2)x + \sqrt{(1-ee^2)x^2 + y^2}} \right], \text{ if } y \leq (1-ee^2)x
\]

and

\[
\lambda = \frac{\pi}{2} - 2\arctan \left[ \frac{(1-ee^2)x}{y + \sqrt{(1-ee^2)x^2 + y^2}} \right], \text{ if } y > (1-ee^2)x
\]

The conventions with regard to the proper quadrant for \(\lambda\) are applied from the signs of \(X\) and \(Y\).

For the height coordinate \(h\), the Euclidean distance between the points \((x, y, z)\) and \((X, Y, Z)\) is used:

\[
\]
Appendix E: Link and description of MATLAB package for simulating flanking structures

Main functions:

*Single_marker_FS_3D.m:* This function simulates the development of flanking structures with a single planar marker around the cutting element. Its inputs are: $W_k$: kinematic vorticity number to determine the flow, $r$: initial viscosity ratio of the cutting element to the ambient medium, $a$: initial shape of the cutting element, $\text{ang}$: initial orientation of the cutting element.

*FlankingStruct1_5markers.m:* This function simulates the development of flanking structures with five linear markers around the cutting element. Its inputs are: $W_k$: kinematic vorticity number to determine the flow, $r$: initial viscosity ratio of the cutting element to the ambient medium, $a$: initial shape of the cutting element, $\text{ang}$: initial orientation of the cutting element.

*Triple_marker_FS.m:* This function simulates the development of flanking structures with three linear markers around the cutting element. Its inputs are: $W_k$: kinematic vorticity number to determine the flow, $r$: initial viscosity ratio of the cutting element to the ambient medium, $a$: initial shape of the cutting element, $\text{ang}$: initial orientation of the cutting element.

*Single_marker_FS.m:* This function simulates the development of flanking structures with a single linear marker around the cutting element. Its inputs are: $W_k$: kinematic vorticity number to determine the flow, $r$: initial viscosity ratio of the cutting element to the ambient medium, $a$: initial shape of the cutting element, $\text{ang}$: initial orientation of the cutting element.

$$h = \sqrt{(X - x)^2 + (Y - y)^2 + (Z - z)^2}$$
vorticity number to determine the flow, \( r \): initial viscosity ratio of the cutting element to the ambient medium, \( a \): initial shape of the cutting element, \( \text{ang} \): initial orientation of the cutting element.

**Other files (sub-functions):**

*Velocity_field_calc5.m*: This function calculates the velocity field along the X-Y cross-section around a 3-D inclusion subjected to a far-field plane strain flow. Its Inputs are \( X \): x-coordinate of the exterior point, \( Y \): y-coordinate of the exterior point, \( a \): initial shape of the cutting element, \( \text{invS} \): inverse of the Eshelby tensor \( S \), \( J_d \): Fourth order identity tensor, \( d \): Strain rate tensor of the far-field flow in terms of cutting element coordinate’s system, \( u_2 \): difference between the cutting element’s strain rate and far-field strain rate, \( \omega \): Vorticity tensor of the far-field flow in terms of cutting element coordinate’s system, \( ll \): Partitioned velocity gradient tensor inside the cutting element.

*Velocity_field_calc_general3D.m*: This function calculates the velocity fields around any 3-D inclusion subject to any far-field flow. Its inputs are \( X \): x-coordinate of the exterior point, \( Y \): y-coordinate of the exterior point, \( Z \): z-coordinate of the exterior point, \( a \): initial shape of the cutting element, \( \text{invS} \): inverse of the Eshelby tensor \( S \), \( J_d \): Fourth order identity tensor, \( d \): Strain rate tensor of the far-field flow in terms of cutting element coordinate’s system, \( u_2 \): difference between the cutting element’s strain rate and far-field strain rate, \( \omega \): Vorticity tensor of the far-field flow in terms of cutting element coordinate’s system, \( ll \): Partitioned velocity gradient tensor inside the cutting element.

*ElliptictoCartesian.m*: This function converts the elliptic coordinates to the respective Cartesian coordinates. Its inputs are \( \xi \) coordinate, \( \eta \) coordinate, \( A \): shape of cutting element. Its outputs are: \( x \): x-coordinate of the exterior point, \( y \): y-coordinate of the exterior point

*CartesiantoElliptic.m*: This function converts the Cartesian coordinates to the respective Elliptical coordinates. Its inputs are \( x \): x-coordinate of the exterior point, \( y \): y-coordinate of the exterior point, \( A \): shape of cutting element. Its outputs are \( \xi \) coordinate, \( \eta \) coordinate.
CartesiantoEllipsoidal.m: This function converts the Cartesian coordinates to the respective Ellipsoidal coordinates. Its inputs are X: x-coordinate of the exterior point, Y: y-coordinate of the exterior point, and Z: z-coordinate of the exterior point, a: shape of the cutting element. Its output is lat: latitude coordinate, long: longitude coordinate, h: height coordinate.

EllipsoidaltoCartesian.m: This function converts the ellipsoidal coordinates to the respective Cartesian coordinates. Its inputs are lat: latitude coordinate, long: longitude coordinate, h: height coordinate, a: shape of the cutting element. Its outputs are: X: x-coordinate of the exterior point, Y: y-coordinate of the exterior point, and Z: z-coordinate of the exterior point

Plot_surface.m: This function plots the flanking structure data in the form of a deformed surface. Its input is ep: a 3×n matrix containing the coordinates of n marker points.

Link for online Github code repository:

https://github.com/ankibues/MOPLA_Application_Matlab/tree/master/Flanking%20Structure%20Investigation/Matlab%20files
Appendix F: Link for supplementary material in Chapter-4

https://github.com/ankibues/MOPLA_Application_Matlab/tree/master/MOPLA_coupling_VPSC/Supplementary%20material
Appendix G: Description of MATLAB files and link for GitHub repository with additional simulated flanking structures and video animations in Chapter-5

*Reverse_modelling_FS.m:* This function reverse deforms a flanking structure, given by linear markers that are digitized using an open-source software WebPlotDigitizer (https://automeris.io/WebPlotDigitizer), for several initial parameters. Its inputs are $X$: $1 \times n$ matrix containing x-coordinates of the digitized markers, $Y$: $1 \times n$ matrix containing y-coordinates of the digitized markers.

*reverse generator.m:* This function generates a velocity gradient tensor corresponding to a reverse far-field flow, required for reverse dynamic modeling in Chapter-5. Its input is $W_k$: kinematic vorticity number of the flow

Link for additional simulated flanking structures:
https://github.com/ankibues/MOPLA_Application_Matlab/tree/master/Flanking%20Structure%20Investigation
Curriculum Vitae

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- Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India
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Publications:


Conferences:
Bhandari A., Jiang D., “A micromechanics-based numerical modeling investigation of flanking structures and its application on determining quantitative kinematic information from ductile shear zones” American Geophysical Union(AGU) Fall Meeting 2020 (Virtual Poster presentation)


Bhandari A., Jiang D., “A multiscale numerical modeling investigation of quartz CPO variation due to flow partitioning”. GeoUtrecht 2020, Utrecht (Oral presentation)


Bhandari A., Jiang D., “A numerical modeling investigation of outcrop-to thin section scale quartz CPO variation observed in nature: Flow field partitioning or Activation of slip system?”, Canadian Tectonic Group Annual Workshop 2018, Saint-Martyrs-Canadiens (Oral presentation).