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The motion of deformable ellipsoids in power-law viscous materials: Formulation and numerical implementation of a micromechanical approach applicable to flow partitioning and heterogeneous deformation in Earth's lithosphere

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ABSTRACT

Earth's lithosphere is heterogeneous in rheology on a wide range of observation scales. When subjected to a tectonic deformation, the incurred flow field can vary significantly from one rheologically distinct element to another and the flow field in an individual element is generally different from the bulk averaged flow field. Kinematic and mechanical models for high-strain zones provide the relations between prescribed tectonic boundary conditions and the resulting bulk flow field. They do not determine how structures and fabrics observed on local and small scales form. To bridge the scale gap between the bulk flow field and minor structures, Eshelby's formalism extended for general power-law viscous materials is shown to be a powerful means. This paper first gives a complete presentation of Eshelby's formalism, from the classic elastic inclusion problem, to Newtonian viscous materials, and to the most general case of a power-law viscous inhomogeneity embedded in a general power-law viscous medium. The formulation is then implemented numerically. The implications and potential applications of the approach are discussed. It is concluded that the general Eshelby formalism together with the self-consistent method is a powerful and physically sound means to tackle large plastic deformation of Earth's lithosphere.

1. Introduction

Rocks are composed of rheologically heterogeneous elements over a wide scale range of observations. When subjected to a tectonic deformation, the incurred flow field in the heterogeneous rock mass is more complex than it would be in a rheologically homogeneous material. In the latter, the flow field varies smoothly in space and usually has a simple relationship with the imposed boundary conditions. In the former, the flow field is more lumpy – varying considerably from one element to another and, to a less degree, within individual elements. As a result, the flow field inside a rheologically distinct element does not in general bear a simple relationship with the far-field tectonic boundary conditions. This presents a major problem to geologists who use deformation structures and fabrics on outcrop and smaller scales ('minor structures' hereafter) to infer deformation boundary conditions on the tectonic scale much larger than the structures themselves (e.g., Simpson and Schmid, 1983; Hanmer and Passchier, 1991).

To simplify the flow field in a heterogeneous body, the normal continuum mechanics approach is to replace the field quantities at a point by their averaged values over a suitable Representative Volume Element (RVE) centered at that point (cf. Batchelor, 2000, pp. 4–5; Ranalli, 1995, pp. 5–6; Lister and Williams, 1983; Li and Wang, 2008, pp. 78–80). This "smoothed-out" and simpler flow field is called the bulk or macroscopic flow field which captures the variation of the flow on the scale greater than the RVE but has no information for smaller (less than RVE) scale complexities in the flow. All current models for high-strain zones, kinematic or mechanical, are ones for the bulk flow field arising from a prescribed boundary condition (e.g., Ramsay and Graham, 1970; Ramberg, 1975; Ramsay, 1980; Sanderson and Marchini, 1984; Simpson and De Paor, 1993; Fossen and Tikoff, 1993; Robin and Cruden, 1994; Dutton, 1997; Jiang and Williams, 1998; Lin et al., 1998; Passchier, 1998; Jiang, 2007c). Minor structures inside natural high-strain zones however are small features compared to the RVE and generally owe their formation to flow field variations on scales below the RVE. Models for the bulk scale flow field cannot be used directly to interpret minor structures.

To understand minor structures we must establish the relationship between the bulk flow field, which can be related to the

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boundary conditions, and flow fields inside individual, rheologically distinct, elements which control the development of observed minor structures. Lister and Williams (1983) described the deviation of the local flow field from the bulk one as "flow field partitioning". We need a physically sound means to govern flow partitioning to bridge the scale gap problem highlighted above.

From a physical point of view, flow field partitioning occurs where there are mechanical interactions between a rheologically distinct element and the surrounding medium. Eshelby (1957, 1959) pioneered a means to deal with such interactions for an isolated elastic region in an infinite elastic field. His approach has since been extended to general viscous materials, linear or power-law, isotropic or anisotropic, and has led to the development of a new and active discipline of continuum mechanics called micromechanics (Mura, 1987; Nemat-Nasser and Hori, 1999; Qu and Cherkaoui, 2006; Hutchinson, 1976; Lebensohn and Tomé, 1993). As will be shown in this paper, Eshelby's inhomogeneity formalism for general power-law viscous materials and the self-consistent method (Kröner, 1961; Hill, 1965, 1966; Hutchinson, 1976; Mura, 1987; Molinari et al., 1987; Lebensohn and Tomé, 1993) provide a powerful means for tackling flow partitioning in natural deformations.

In this contribution, I first give a complete presentation of Eshelby's formalism, from the classic elastic inclusion problem, to Newtonian viscous materials, and to the most general case of a power-law viscous inhomogeneity embedded in a power-law viscous medium. I then implement the formulation numerically for practical use. Mathcad worksheets are provided in the online supplementary data for interactive numerical simulation and result visualization. To make the paper less dependent on the materials science literature so that the reader can follow the flow of ideas more easily, I have reproduced some published equations in some detail. Finally I discuss the implications and potential applications of the approach in geology. A full account of the self-consistent formulation and its implementation will be presented in a separate contribution.

2. Nomenclature

Throughout this paper, I will use a combination of Cartesian tensor notation and a standard tensor/matrix notation. Tensors are represented by bold-face letters. Fourth order tensors will be represented by uppercase bold-face letters. As far as possible, second order tensors will be represented by lowercase bold-face letters. A few exceptions are made for some tensors to be consistent with commonly used notations in earlier papers. Scalars and scalar components of tensors are represented by italic letters. The summation convention is assumed unless declared otherwise whereby a repeated index represents summation over the value of 1, 2, 3 for the index. The double contracted product of two tensors is denoted by ':'. Thus the *ijkl*-components of **A**:**B**, where both **A** and **B** are fourth order tensors, are $A_{ijmn}B_{mnkl}$, the *ij*-components of **A**:**b**, where **b** is a second order tensor, are $A_{ijmn}b_{mn}$, and **a**:**b** is a scalar, $a_{ij}b_{ij}$. The product between 2 s order tensors or between two matrices is denoted as **ab**, with *ij*-components being $a_{ik}b_{kj}$.

The following three fourth order unit tensors are used in this paper:

$$J_{ijkl} = \delta_{ik}\delta_{jl},\ J^{S}_{ijkl} = \frac{1}{2}\left(J_{ijkl}+J_{jikl}\right),\ J^{A}_{ijkl} = \frac{1}{2}\left(J_{ijkl}-J_{jikl}\right)$$

where $\delta_{ij}=1$ for $i=j$ and 0 for $i \neq j$. The three tensors $\mathbf{J}, \mathbf{J}^{S}$, and $\mathbf{J}^{A}$ are referred to, respectively, as the fourth order unit tensor, the fourth order symmetric unit tensor, and the fourth order anti-symmetric unit tensor (Li and Wang, 2008, p, 8).

a_1, a_2, a_3, a_i the semi-axes of an ellipsoid (first, second, third, general)
$\mathbf{A}$ strain rate partitioning tensor (fourth order)
$\mathbf{b}^1, \mathbf{b}^2, \mathbf{b}^3, \mathbf{b}^4, \mathbf{b}^5, \mathbf{b}^6, \mathbf{b}^\lambda$ base set of 6 orthonormal symmetric second-order tensors, ($\lambda = 1, 2, \dots 6$)
$\mathbf{C}, \mathbf{C}_{\text{inh}}, \mathbf{C}_{\text{M}}$ elastic moduli tensor (general, of the inhomogeneity, of the matrix medium)
$\mathbb{C}$ 6×6 matrix of the elastic moduli
δt time step for numerical computation
D^{axis} diagonal matrix of the strain rates for the three semi-axes of an ellipsoid
$\mathbf{e}, \mathbf{e}^{\text{C}}, \mathbf{e}^{*}, \mathbf{e}^{\text{M}}, \mathbf{e}^{\text{inh}}, \tilde{\mathbf{e}}$ elastic strain tensor (general, constrained, eigen-, in the far-field matrix medium, in an inhomogeneity, difference between the inhomogeneity and the far-field matrix medium)
$E(\theta,k)$ elliptic integral of the second kind
$\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^{\text{inh}}, \boldsymbol{\varepsilon}^{E}\ \boldsymbol{\varepsilon}^{\text{M}}, \boldsymbol{\varepsilon}^{0}, \tilde{\boldsymbol{\varepsilon}}$ viscous strain rate tensor (general, of an inhomogeneity, of an ellipsoid, of the matrix medium, back-extrapolated term in tangent linearization, difference between the ellipsoid and the far-field matrix medium)
$F(\theta,k)$ elliptic integral of the first kind
$\mathbf{H}, \widehat{\mathbf{H}}$ Hill's constraint tensor, its inverse (also known as the interaction tensor)
$\mathbf{I}$ second order unit tensor
$\mathbf{J}, \mathbf{J}^{\text{S}}, \mathbf{J}^{\text{A}}$ 4th order unit tensor (general, symmetric, anti-symmetric)
$\mathbb{J}$ the *J*-integrals in calculation of Eshelby tensors
$\mathbf{L}$ velocity gradient tensor of matrix flow (second order)
$\mathbf{M}, \mathbf{M}_{\text{M}}, \mathbf{M}_{\text{inh}}, \mathbf{M}^{(\tan)}, \mathbf{M}^{(\sec)}$ 4th order viscous compliances tensor (general, of the matrix medium, of the inhomogeneity, tangent, secant)
$\underline{\mathbf{Q}}$ matrix defined by the orientation of an ellipsoid
$\boldsymbol{\Theta}$ angular velocity tensor of an ellipsoid
$\theta_1, \phi_1, \theta_2$ spherical angles defining the orientation of an ellipsoid
n, n_{M} stress exponent (general, of the matrix material)
r, r_{eff}, r_0 viscosity ratio between ellipsoid and matrix medium (Newtonian, effective where one or both the ellipsoid and the matrix medium are power law, effective at the matrix medium strain rate state
$\boldsymbol{\sigma}, \boldsymbol{\sigma}^{\text{inh}}, \boldsymbol{\sigma}^{\text{M}}, \tilde{\boldsymbol{\sigma}}$ Cauchy stress tensor (general, in the inhomogeneity, in the matrix medium, difference between the inhomogeneity and the matrix medium)
$\mathbf{S}, \boldsymbol{\Pi}$ symmetric Eshelby tensor, anti-symmetric Eshelby tensor
$\mathbf{T}, \mathbf{T}^{\text{S}}, \mathbf{T}^{\text{A}}$ 4th order Green interaction tensor, symmetric Green interaction tensor, anti-symmetric Green interaction tensor
$\mathbf{w}^{\text{inh}}, \mathbf{w}^{\text{E}}, \mathbf{w}^{\text{M}}, \tilde{\mathbf{w}}$ vorticity in an inhomogeneity, in an ellipsoid, in the far-field matrix medium, vorticity difference between the ellipsoid and the far-field matrix medium
$\boldsymbol{\omega}^{\text{inh}}, \boldsymbol{\omega}^{\text{M}}$ elastic rotation tensor in the inhomogeneity, elastic rotation tensor in the remote matrix medium
ω incremental angle of rotation
$\hat{\boldsymbol{\omega}}$ normalized incremental angular rotation tensor

3. The interaction between an elastic inclusion/inhomogeneity and the embedding infinite elastic medium: the classic Eshelby formalism

Eshelby (1957, 1959) considers the elastic field of an infinite uniform elastic body caused by a "region" he called "inclusion"