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Patterns of strain localization in heterogeneous, polycrystalline rocks – a numerical perspective

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ABSTRACT

The spatial and temporal patterns of strain localization in materials with pre-existing heterogeneities are investigated via a series of two-dimensional numerical models. Models include (i) a dynamic feedback process, to simulate rheological weakening in response to the transition from non-linear flow (dislocation creep) to linear flow (diffusion creep/grain boundary sliding), and (ii) a time dependent strengthening process, counteracting the weakening process. Different load bearing framework geometries with 20% weak component are used to evaluate the impact of geometry on the strength of the material and its ability to localize strain into an interconnected weak layer (IWL). Our results highlight that during simple shear, if dynamic weakening with or without strengthening feedbacks is present, strain is quickly localized into an IWL, where an increasing proportion of weak material increases the interconnections between the IWLs, thereby increasing the anastomosing character of the shear zones. We establish that not only bulk strain localization patterns but also their temporal patterns are sensitive to the dominance of the weakening or strengthening process. Consequently, shear zones are dynamic in time and space within a single deformation event. Hence, the pattern of finite strain can be an incomplete representation of the evolution of a shear zone network.

1. Introduction

Strain localization fundamentally controls a material's rheological response to deformation. Shear zone initiation and development is, therefore, widely studied at all scales, from single crystal behavior to crustal scale high strain zones (e.g. Carreras, 2001). There is well-documented evidence of the major role localization plays in governing important rheological and economic structures (e.g. Bouchot et al., 1989). However, speculation remains regarding the mechanisms and patterns of strain localization, including the influence of rheology and geometry of pre-existing heterogeneities, and the importance of weakening and strengthening processes. For example, field evidence indicates strain concentration is highly variable, from single zones of ultramylonite to mylonite, to anastomosing, that is, interconnected, sets of high strain zones (e.g. Arbaret et al., 2000; Carreras et al., 2010; Svahnberg and Piazolo, 2010). Understanding the underlying principles for this variability will improve our ability to utilize shear zone localization patterns for characterization of material behavior through time and to model Earth processes.

Rock heterogeneity impacts strength anisotropy, the bulk strength and the evolution of the fabric governing where localization occurs. Heterogeneity results from the (i) strength contrast between the phases (e.g. Dell'Angelo and Tullis, 1996; Handy, 1994; Hansen et al., 2012; Holyoke III and Tullis, 2006); (ii) interconnectivity, and geometric patterns of weak components (e.g. Gerbi, 2012; Gerbi et al., 2016; Treagus, 2002; Tullis et al., 1991); (iii) pre-existing fabrics, for example, foliation (e.g. Montési, 2013; Rennie et al., 2013) and brittle fractures (e.g. Segall and Simpson, 1986); (iv) volume fraction of weak components (e.g. Handy, 1994; Shea and Kronenberg, 1993; Takeda and Griera, 2006; Treagus, 2002); and (v) deformation mechanisms active in each phase (e.g. Dell'Angelo and Tullis, 1996; Holyoke III and Tullis, 2006).

Strength anisotropy can also evolve by (i) fluid ingress and egress, with or without reactions, creating weaker phases (e.g. Finch et al., 2016; Holyoke III and Tullis, 2006), (ii) changes in temperature, perhaps due to shear heating (e.g. Hobbs et al., 2008; Platt, 2015; Poulet et al., 2014), and/or (iii) recrystallization, causing grain size reduction (e.g. Drury, 2005; Warren and Hirth, 2006) and/or grain coarsening (e.g. De Bresser et al., 1998). Both

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strengthening and weakening by grain size reduction and growth processes (e.g. Herwegh and Berger, 2004) and water transfer (Finch et al., 2016) have been shown to occur simultaneously in a shear zone. Such coupled and competing processes are known to be important in the Earth's crust, changing the underlying deformation processes as the balance between the processes changes (e.g. Chester, 1995; De Bresser et al., 1998).

Numerical models of evolving strength anisotropy due to grain size changes have been used to explore strain localization. Jessell et al. (2005) implement grain size reduction and growth processes resulting in rheological softening and hardening, respectively. In contrast, Cross et al. (2015) use a grain size paleopiezometer to drive the balance between grain size growth and reduction to a steady state grain size, while Herwegh et al. (2014) implement a dynamic transition between grain size insensitive and sensitive flow regimes using a paleowattmeter. Other authors (e.g. Jessell et al., 2009; Mancktelow, 2002; Takeda and Griera, 2006) have implicitly modeled strength variation using viscosity as a proxy for grain size.

In this contribution, we take a numerical approach and investigate the local dynamic feedback between weak and strong components, using stress dependent weakening and time dependent strengthening as a proxy, rather than explicitly defining a particular strengthening or weakening process. We examine how this dynamic feedback process can readily cause an initially load bearing framework (LBF), where the weak phase is surrounded by a strong matrix, to form an interconnected weak layer (IWL) parallel to the shear plane. In contrast to Handy (1994), who used the IWL and LBF as end member geometries, the numerical models used here show a dynamic feedback process can readily create an IWL from a LBF. We find the IWLs interconnect where the weakening process is widespread, that is, the anastomosing character of the shear zones increases. Even though the processes responsible for weakening and strengthening may operate at the grain scale, our model describes patterns that can be applied up to km-scale localization.

2. Numerical set-up

2.1. General model

Elle, an open source numerical simulation platform (Bons et al., 2008), is used to model deformation of a two-dimensional structure undergoing dextral simple shear. In the Elle platform multiple processes may act sequentially upon the numerical 2D structure (Supp. Fig. 1a). Here, processes include viscous deformation and/or rheological weakening and/or rheological hardening. The viscous deformation of the model is handled in the finite element method (FEM) code, Basil (Houseman et al., 2008). The 2D structure consists of two layers of information. Layer 1 records polygon geometry (Fig. 1a(i)) where each polygon is defined by a closed loop of boundary nodes connected by straight segments (Supp. Fig. 1b). Physical properties including viscosity pre-factor, viscous flow law are defined for each polygon. Cumulative and instantaneous strain and stress are recorded as the simulation progresses. In contrast to many previous applications of the Elle platform (e.g. Llorens et al., 2016; Piazolo et al., 2002), each polygon represents an area of similar physical properties rather than a specific grain, such that straight segments between boundary nodes should not be considered as grain boundaries. Layer 2 is an initially 100×100 square grid mesh of unconnected nodes or material information points (Supp. Fig. 1b). In this implementation, the Layer 2 of unconnected nodes provides passive markers of the deformation field as the model run progresses (e.g. Jessell et al., 2009).

A complete simulation includes defining a starting polygon geometry or rock structure, then cycling the rock structure through the series of processes that includes the Basil deformation step, to a user defined incremental strain, and may include none, one, or both of the two optional dynamic rheological processes (i.e. weakening, hardening, see Supp. Fig. 1a) until the desired finite shear strain is reached.

In the simulations presented here, a full iteration of the Elle cycle includes passing the 2D structure to the FEM code Basil (Houseman et al., 2008) where the Layer 1 polygons are triangulated into a finer mesh for the FEM deformation step. Dextral simple shear is applied, using boundary conditions of constant displacement of +0.025 (at the top boundary) and −0.025 (at the bottom boundary). Boundaries are defined to be periodic in both the x and y direction. In this implementation Basil uses dimensionless variables and assumes an incompressible medium with viscous behavior described by the constitutive relationship:

$$\tau_{ij} = 2\eta\dot{\varepsilon}_{ij} = \eta\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right]$$

where τ_{ij} is the deviatoric stress tensor, $\dot{\varepsilon}_{ij}$ is the strain rate tensor, u is the velocity in the x or y direction, η is the effective viscosity defined by:

$$\eta = \frac{1}{2}\eta^{*}\dot{E}^{\left(\frac{1-n}{n}\right)}$$

where $\dot{E}$ is the second invariant of the strain rate tensor, n is the stress exponent and η^{*} is a viscosity pre-factor. The FEM code Basil, calculates a converged solution based on the constitutive relationships, boundary conditions and the Layer 1 polygon geometry and properties input from Elle. For a full discussion of the Basil formulation, please see Houseman et al. (2008).

The solution calculated by Basil is passed back to Elle where the geometry and values (e.g. stress) of Layer 1 polygon mesh and the position of the Layer 2 nodes are both updated. The Elle control script then calls the next process to act upon the structure (Supp. Fig. 1a). To simulate the processes of weakening and strengthening during deformation, Elle calls each process in turn, at each time step (Jessell et al., 2001; Piazolo et al., 2010), depending on the chosen simulation set, as outlined below.

Within Elle, the initial viscosity pre-factor and stress exponent are defined on the Layer 1 polygons, hence, it is possible to define geometries with differing properties on each polygon. The properties are dimensionless, based on the unit cell. For the presented numerical models, we have defined a load bearing framework (LBF) where approximately 20 area% is rheologically weak, with a relatively low viscosity pre-factor of 1, while the majority of the polygons are stronger, with viscosity pre-factor of 5. We present results using five different initial geometries (Fig. 1a(ii)–(iv)); random, clusters, rings and two with stripes, the first where the stripes are parallel to the shear plane, here called horizontal stripes, and the second where the stripes are perpendicular to the shear plane, here called vertical stripes. We run four sets of simulations which differ in the complexity of dynamic feedbacks simulated. Simulation set I does not involve any dynamic feedbacks, hence no rheological changes occur throughout the deformation. In contrast, simulation sets II and III involve dynamic weakening (Fig. 1c) while in simulation set IV both weakening and strengthening are modeled (Fig. 1d). A summary of the simulations undertaken is included in Table 1 and the dynamic simulations are visually represented in Fig. 1b.

All simulations are run to 80 simulation steps, representing finite shear strain (γ) of 2. One simulation set is additionally run to a finite shear strain of 2.75 to allow assessment of the effect of higher finite strain on material strength behavior. Stress (σ) and incremental strain values ($\varepsilon_{\mathrm{Incr}}$) are calculated from velocity gradients during the deformation step in Basil (for details,