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ABSTRACT

It has been debated for decades whether rigid inclusions, such as porphyroclasts and porphyroblasts, do or do not rotate in a softer matrix during deformation. Experiments and numerical simulations with viscous matrix rheologies show ongoing rotation of circular inclusions, whereas using Mohr-Coulomb plasticity results in nonrotation. Because the rocks in which inclusions are found normally undergo deformation by dislocation creep, we applied a full-field crystal plasticity approach to investigate the rotation behavior of rigid circular inclusions. We show that the inclusion's rotation strongly depends on the anisotropy of the matrix minerals. Strongly anisotropic minerals will develop shear bands that reduce the rotation of inclusions. Inhibition of rotation can only occur after a significant amount of strain. Our results may help to explain why geologic rigid objects often show evidence for rotation, but not necessarily in accordance with the viscous theory that is usually applied to these systems.

INTRODUCTION

The kinematics of rigid inclusions (such as porphyroblasts and porphyroclasts) embedded in a deforming ductile matrix are subject to ongoing debate (Bell et al., 1992; Passchier et al., 1992; Fay et al., 2008; Bons et al., 2009; Johnson, 2009, 2010; Sanislav, 2010). Most of this debate has concentrated on the question: Does a rigid inclusion rotate with respect to an external reference frame? This is not a trivial question. For example, whereas most authors would regard spiraling inclusion patterns in "snowball" garnets as indicating rotation of the garnet during a single noncoaxial shearing event (e.g., Schoneveld, 1977; Passchier et al., 1992), others interpret these patterns as indicating a series of distinct deformation events (e.g., Bell, 1985; Bell et al., 1992, 1998). A correct understanding of rigid object rotation is therefore of crucial importance in unraveling deformation histories (shear sense, vorticity, amount of strain, etc.) of deformed rocks and ancient orogenies.

Most of the theoretical, experimental, and numerical investigations to date (e.g., Ghosh and Ramberg, 1976; Ferguson, 1979; Marques and Burlini, 2008; Fletcher, 2009) have concluded that a rigid inclusion rotates according to the analytical solution of Jeffery (1922) and Ghosh and Ramberg (1976). This solution applies to rigid ellipsoidal inclusions in a linear viscous matrix. Two-dimensional simulations by Bons et al. (1997) have shown that the rotation rate is the same for power-law matrix rheologies. Recently, the analytical solutions of Fletcher (2009) demonstrated that this is also valid for a homogeneous anisotropic viscous matrix. However, several factors have been recognized that may inhibit rotation or even induce a rotation rate in an opposite sense, including: slip and/or decoupling between the matrix and inclusion interface (e.g., Ildefonse and Mancktelow, 1993; Ceriani et al., 2003; Schmid and Podladchikov, 2005), confined flow because a shear zone is thin compared to the inclusion size (Marques and Coelho, 2001; Biermeier et al., 2001), interaction between multiple inclusions (Ildefonse et al., 1992; Jessell et al., 2009), or strain localization in the matrix (ten Grotenhuis et al., 2002; Fay et al., 2008). Most of these factors are expected to play a role under geological conditions and have been considered to characterize the flow of shear zones (Marques et al., 2007; Johnson et al., 2009a, 2009b) and to explain porphyroclast orientations that are not consistent with the analytical solution (ten Grotenhuis et al., 2002).

Most experiments and numerical simulations use (linear) viscous matrix rheologies, which, of course, give results consistent with analytical solutions for the same case. The question is whether a homogeneous, isotropic viscous rheology is applicable to real rocks. Natural rocks are typically crystalline, displaying heterogeneities and showing an anisotropic mechanical behavior, which will favor heterogeneous stress and strain rate fields and the possibility of strain localization. Bell (1985) therefore argued that the formation of anastomosing localized shear bands would completely inhibit rotation of rigid objects. Use of a Mohr-Coulomb–type plasticity indeed leads to localization of strain around rigid objects and reduces rotation of the objects (ten Grotenhuis et al., 2002). It is, however, questionable whether Mohr-Coulomb plasticity is appropriate for rocks that typically deform by dislocation creep mechanisms and would exhibit a power-law viscous rheology (e.g., Kirby and Kronenberg, 1987).

In this paper, we will show that the strain localization that results from stress and strain rate heterogeneities in a polycrystalline aggregate that deforms by dislocation creep does affect the rotation rate of embedded rigid objects. We will show that the rotation rate of objects is less than that predicted by Jeffery (1922), but not completely inhibited as suggested by Bell (1985; e.g., Fay et al., 2008, and references therein).

NUMERICAL METHOD

We used two-dimensional numerical modeling to investigate the rotation of a rigid inclusion that is embedded in an anisotropic polycrystalline matrix. The numerical approach is based on the coupling of a full-field viscoplastic formulation based on the fast Fourier transform (FFT; Lebensohn, 2001), and a front-tracking approach using the numerical platform *Elle* (e.g., Bons et al., 2008). Briefly, the FFT formulation provides an exact solution of the micromechanical problem by finding a strain rate and stress field, associated with a kinematically admissible velocity field, that minimizes the average local work-rate under the compatibility and equilibrium constraints (see Lebensohn [2001] and Lebensohn et al. [2008] for a detailed description of the method). The numerical platform *Elle* is an open-source software for the simulation of the evolution of microstructures during deformation and metamorphism. Previously, *Elle* has been used to simulate several microstructure processes, such as grain growth (Bons et al., 2001; Jessell et al., 2003), dynamic recrystallization (Piazolo et al., 2002), strain localization (Jessell et al., 2005), or melt processes (Becker et al., 2008), among other examples.

Since both codes use periodic boundary conditions and physical space is discretized into a regular array of nodes (or Fourier points), a direct one-to-one mapping between the data structures of both codes is possible. Grain boundaries are explicitly simulated using a vector layer that defines microstructure from a compilation of nodes and boundary segments. The numerical simulation is achieved by iterative application of small time steps of each process in turn. High strains, as observed in nature, can be attained using the periodic model boundaries and the use of a particle-in-cell approach.

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The anisotropic crystalline behavior is defined using a nonlinear viscous rate-dependent approach, where deformation at the grain scale is assumed to be accommodated by dislocation glide only (e.g., Lebensohn, 2001). A hexagonal symmetry mineral was chosen to simulate the mechanical properties of the polycrystal, and deformation was allowed to be accommodated mainly by glide along a basal plane and minor slip on nonbasal systems (i.e., pyramidal or prismatic planes). The results are applicable to any mineral that exhibits a marked anisotropy (e.g., low-temperature quartz). The resistance of slip systems is simulated by means of the critical resolved shear stress. Here, the grain anisotropy (M) parameter is characterized as the ratio between the critical stresses of the nonbasal and basal slip systems (e.g., Lebensohn, 2001). Stress exponents $n = 2$ and $n = 3$ were used, and the same value of n was assumed for all slip systems. The mechanical behavior of the inclusion was simulated using the same approach but with a single critical stress for all slip systems that was set at 50 times the critical stress for basal slip in the matrix crystals. The initial model consisted of a single circular inclusion in a matrix of 250 grains with randomly assigned Euler angles for their lattice orientation (Fig. 1A).

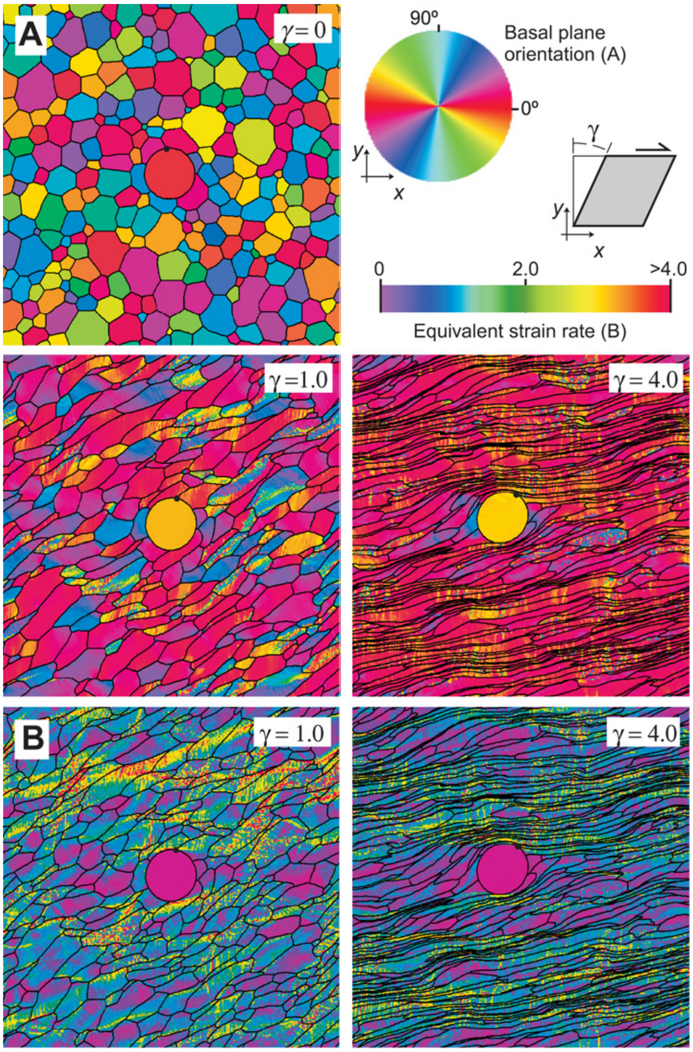

Figure 1. A: Evolution of microstructure and grain boundary map for simulation with grain anisotropy M = 10 and stress exponent n = 2. Colors indicate orientation of basal plane with respect to horizontal shear plane. B: Evolution of strain rate field normalized to bulk strain rate. As deformation increases, strain distribution evolves from local intracrystalline high-strain bands to a network of high-strain bands subparallel to shear plane. Black dot indicates rotation of inclusion.

Additionally, a fine-grained simulation with 64,000 grains was done to test the effect of the matrix's grain size. A resolution of 256 × 256 Fourier points was used to map lattice orientations, resulting in a unit cell defined by 65,536 discrete nodes. Dextral simple shear up to a shear strain of γ = 5 parallel to the x-axis was applied using velocity boundary conditions.

RESULTS

An example of numerical results for the M = 10 and n = 2 model is shown in Figure 1. At low strain, a shape preferred orientation (SPO) of grains parallel to the maximum finite extension direction is observed. Strain distribution becomes increasingly heterogeneous with progressive strain. Synthetic shear bands with extremely stretched grains develop that bound lozenge-shaped low-strain domains. The strain partitioning that is visible from the grain shapes is also visible in maps of the equivalent strain rate (ratio between local and bulk strain rate; Fig. 1B). Strain rate is highly variable, with local strain rates up to eight times higher than the bulk strain rate. At low strain, deformation is concentrated in intracrystalline bands that progressively connect and evolve into intercrystalline shear bands. High-strain zones wrap around the inclusion, with the development of strain shadows and a sigma-clast geometry.

Strain localization is governed by the anisotropic viscoplastic behavior of the crystalline material. With increasing strain, a strong lattice preferred orientation (LPO) develops, with reorientation of the basal planes subparallel to the shear plane. This LPO weakens the material as the easy-slip plane is oriented parallel to the shear plane.

Inclusion Rotation Rate

The influence of strain partitioning on the behavior of the inclusion was explored by modifying the grain anisotropy parameter M. M = 1 represents the case where all the slip systems have the same critical resolved shear stress, making the single-crystal case relatively isotropic. Increasing M enhances the heterogeneous response of the aggregate. For simple shear, the analytical solution of Jeffery (1922) predicts that a circular inclusion will rotate synthetically to the shear sense at a constant rotation rate equal to half the shear strain rate. Our simulations show that at M = 1, the inclusion indeed behaves as predicted by Jeffery (1922) (Fig. 2A). With increasing M, rotation rates increasingly deviate from the analytic solution—the inclusion essentially does not rotate after a shear strain of one in a highly anisotropic matrix (M = 10). Similar tendencies are observed for n = 2 and n = 3 simulations, although an increase in nonlinearity creates larger deviations in the rotation rate. Note that at low shear strains, all simulations show a roughly constant rotation rate similar to the theoretical model.

The difference in rotation behavior is clearly related to the amount of strain partitioning, which strongly increases up to $M \approx 10$ (Fig. 3). For isotropic and low-anisotropic cases (M ~ 1–2), deformation is mainly homogeneous, and only minor strain localization is observed surrounding the inclusion. The flow pattern is equivalent to that observed in homogeneous isotropic viscous matrices (Bons et al., 1997; Schmid and Podladchikov, 2005). Increasing M increases the heterogeneities at grain scale and accelerates the development of an intercrystalline network of shear bands, which become thinner at high values of M. The growth of this network causes a decrease of the shear strain rate transmitted to the inclusion, which reduces its rotation rate (Fig. 2A).

Variations in Rotation Rate

The results show that the development of shear bands has a strong control on the rotational behavior of rigid inclusions. Different distributions of shear bands are thus expected to result in different amounts of rotation. This was tested by running four identical simulations with M = 10. The only difference between the simulations was the initial random distribution of lattice orientations in the matrix grains. After a shear strain

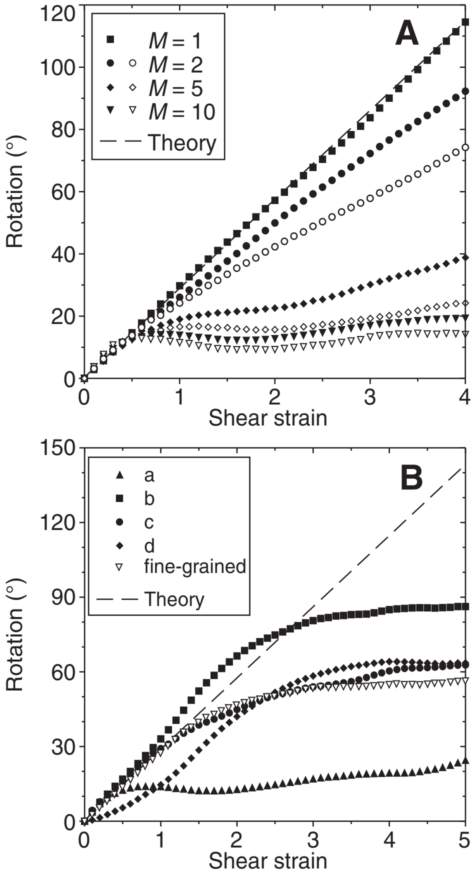

Figure 2. A: Evolution of finite rotation for a range of grain anisotropies (M). Filled symbols are simulations with n = 2, while white symbols are for n = 3. All simulations were run with same initial microstructure. Jeffery's (1922) theoretical solution is shown as a dashed line. B: Evolution of finite rotation with shear strain for four random coarse-grained simulations (a–d) and a fine-grained simulation. Grain anisotropy was set at M = 10 in all simulations.

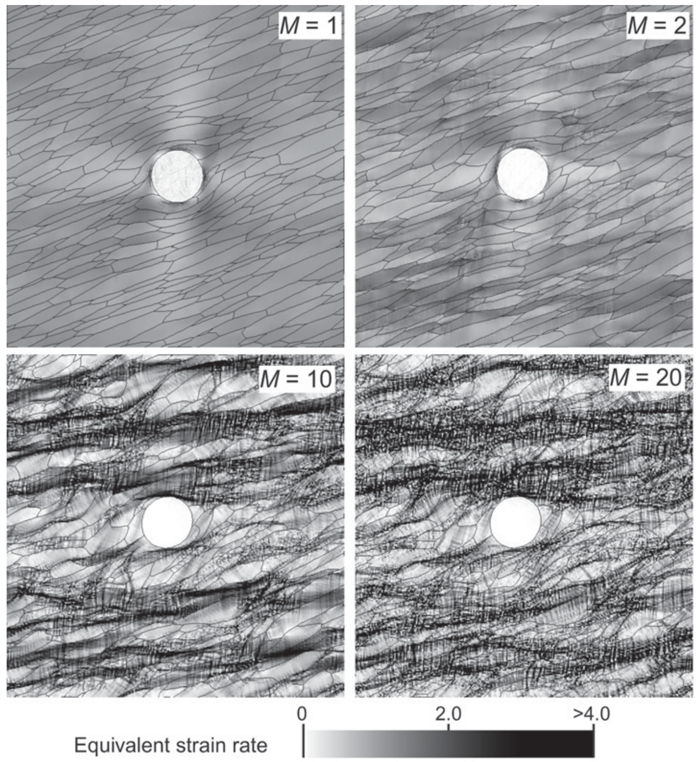

Figure 3. Maps of equivalent strain-rate field normalized to bulk strain rate for different values of grain anisotropy M. Stress exponent was n = 2 for all simulations. All plots are after a finite shear strain of two.

of 4.0, all simulations show a similar pattern of anastomosing high-strain zones separating low-strain regions. However, the inclusion's rotation history and final orientation strongly vary among the simulations (Fig. 2B). Although there is a general tendency toward nonrotation, the shear strain needed can vary strongly (γ = 0.5–3), as does the finite rotation angle (~15°–85°). Fine-grained simulations showed similar tendencies, with the development of stable orientations and the deviation of the final orientation with respect to analytical solutions.

DISCUSSION AND CONCLUSIONS

Our observations show that the rotational behavior of rigid inclusions, such as porphyroblasts and porphyroclasts, is strongly influenced by the localization of strain on the scale of the inclusion. Other workers have investigated this effect by enforcing localization through the introduction of a weak layer or a slipping surface around the inclusion (e.g., Ceriani et al., 2003; Schmid and Podladchikov, 2005) or by using Mohr-Coulomb plasticity (ten Grotenhuis et al., 2002; Fay et al., 2008). Although these studies had their merit in showing the effect of strain localization, they do not well represent the actual physical processes that operate in the system. Our simulations have the advantage that the constitutive behavior of our model material better resembles that assumed for real deforming geological materials. As a result, strain localization develops spontaneously and as a function of strain, rather than being absent or enforced to occur at a certain sites, such as the surface of the inclusion.

Our simulations indicate that rigid inclusions would rotate during noncoaxial deformation. Low-anisotropy (low M) matrices do not develop strong strain localization, and the rotation of inclusions approximately follows the predicted rate of Jeffery (1922). Strong strain localization occurs in high-anisotropy (high M) materials, in which case rotation is inhibited once shear bands are established. A significant difference with the numerical model of Fay et al. (2008) is that strain localization is instantaneous if Mohr-Coulomb plasticity is used, whereas it requires an amount of strain to develop in our crystal plastic rheological model. The development of shear bands does therefore lead to the reduction or complete inhibition of rotation of rigid inclusions, as already proposed by Bell (1985) and coworkers. However, the stalling of rotation only occurs after a significant amount of strain, and objects can rotate by a significant amount (up to 90°).

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