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Numerical simulations of texture development and associated rheological anisotropy in regions of complex mantle flow

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[1] The development of Lattice Preferred Orientations (LPO) within olivine aggregates under flow in the upper mantle leads to seismic and rheological (or viscoplastic) anisotropies. We compare predictions from different micromechanical models, applying several commonly used theoretical descriptions to an upwelling flow scenario representing a typical oceanic spreading center. Significant differences are obtained between models in terms of LPO and associated rheology, in particular in regions where the flow direction changes rapidly, with superior predictions for the recently proposed Second-Order approach. This highlights the limitations of ad hoc formulations. LPO-induced rheological anisotropy may have a large effect on actual flow patterns with 1–2 orders of magnitude variation in directional viscosities compared to the isotropic case. **Citation:** Castelnau, O., D. K. Blackman, and T. W. Becker (2009), Numerical simulations of texture development and associated rheological anisotropy in regions of complex mantle flow, *Geophys. Res. Lett.*, *36*, L12304, doi:10.1029/2009GL038027.

1. Introduction

[2] The aim of this study is to compare the predictions of different polycrystal models (based on micromechanical approaches) that have been employed to study mineral alignment during flow in the upper mantle. Computational capabilities are reaching a point where the potential rheological effects of such Lattice Preferred Orientation (LPO) can be considered, e.g., by a full coupling of those models with large scale flow models (in this paper we use the term “rheology” to describe the *viscoplastic* behavior). In order to have confidence in taking this next step, the detailed behavior of the different micromechanical models used for LPO evolution and associated rheology needs to be understood. Although models most commonly in use today have been partly tested against available experimental data and field constraints for simple deformation paths, a systematic assessment of how they compare when subjected to more complex deformation paths has not been reported. A number of previous studies considered finite strain as a proxy for LPO development [see, e.g., *Hall et al.*, 2000; *Becker et al.*, 2003]. Micromechanical models, which aim at bridging LPO development with single grain behavior, have been introduced in the early ’90s [*Ribe and Yu*, 1991; *Chastel et al.*, 1993; *Tommasi et al.*, 2000; *Dawson and Wenk*, 2000; *Kaminski et al.*, 2004; *Mühlhaus et al.*, 2004] and some of them have been applied to large scale flow modelling [e.g., *Becker et al.*, 2006].

[3] An important consequence of LPO development is the associated anisotropy of the mechanical properties. However, most published studies only address the *elastic* anisotropy, probably because of its link with the observed seismic anisotropy. The link between local deformation mechanisms at the grain scale, the overall flow stress of the mantle, LPO development, and rheological anisotropy has received much less attention, although it may have a notable influence on regional and global convective flow pattern [*Christensen*, 1987; *Blackman*, 2007; *Lev and Hager*, 2008a]. We address in the following the predictive capability of several rheological models, all of them based on micromechanical modeling, with an eye toward their eventual use in coupled LPO-geodynamic flow simulations.

2. Micromechanical Modeling

[4] The main ingredient of all micromechanical models used to reproduce or predict LPO development in peridotites is the localization law, which basically describes how stress and strain-rates are distributed among the different grains of the polycrystalline specimen. Grains may be favourably or unfavourably oriented to promote plastic deformation, due to the mechanical interactions with neighboring grains and the available slip systems for dislocations. With the localization law in hand, polycrystal rheology can be estimated for a given LPO, and LPO development can be determined straightforwardly at large plastic strain. A puzzling feature of olivine plasticity is the limited number of independent slip systems for the dislocations. None of the observed slip systems allows an axial deformation of the crystal lattice along the *a*, *b*, and *c* lattice directions, leaving olivine crystals with only three independent slip systems. This is known to be insufficient for a polycrystal to deform. Five independent slip systems would be required according to the von Mises rule, but it has been shown recently that four systems are in fact sufficient [*Castelnau et al.*, 2008a, 2008b]. Therefore, taking into account additional deformation mechanisms such as dislocation climb, grain boundary sliding, or diffusion creep, is necessary and critical since the resistance of these accommodation processes entirely controls the flow stress of the polycrystal. This difficulty has been largely neglected or bypassed up to now.

[5] Evaluating the interaction between deforming grains is a complex mechanical problem. Among models already

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applied to the upper mantle, a simple solution is provided by the static model [*Reuss*, 1929] which assigns the stress in individual grains to be that experienced by the polycrystal as a whole. The advantage of this model is its simplicity, but this comes at the expense of its limited physical relevance. Indeed, this model incorrectly predicts that olivine polycrystals can deform with a single slip system. More accurate predictions can be obtained with the *Self-Consistent* (SC) estimate [*Kröner*, 1978]. For *linear* viscosities, this model predicts the exact polycrystal behavior when the grain geometrical arrangement exhibits some specific statistical properties [*Milton*, 1985]. A great advantage of the SC scheme is that it accounts for the heterogeneity of stress and strain-rate inside grains, as evidenced experimentally (L. Xu and B. Evans, Strain heterogeneity in deformed carrara marble using a micro-scale strain mapping technique, submitted to *Journal of Geophysical Research*, 2009), in contrast to all other methods applied up to now to peridotites. The extension of the SC theory to non-linear viscoplasticity induces several technical difficulties, one of them being a linearization of the polycrystal [*Ponte Castañeda and Suquet*, 1998] that can critically affect the results, in particular the predicted overall flow stress. A robust linearization method has been proposed only recently, leading to the *Second Order Self-Consistent* (SO) model [*Ponte Castañeda*, 2002] that has been shown to provide qualitative and quantitative agreement with several "exact" numerical solutions, e.g., for fiber-reinforced composites [*Idiart et al.*, 2006] and various polycrystals [*Lebensohn et al.*, 2007] including olivine [*Castelnau et al.*, 2008a, 2008b]. For example, the SO model correctly predicts that four independent slip systems are necessary, and sufficient, for olivine to deform. The *Tangent Self-Consistent* (TGT) model [*Molinari et al.*, 1987; *Lebensohn and Tomé*, 1993] used in a number of geophysical studies (and usually referred to as the "VPSC model") can be considered as an approximation of the more general SO formulation. Its formulation suffers from significant inconsistencies [*Masson et al.*, 2000] leading to the incorrect prediction of a finite polycrystal viscosity when grains exhibit only three independent slip systems [*Castelnau et al.*, 2008a, 2008b].

[6] Although these models (and particularly the SO model) efficiently condense the very large complexity of the mechanical problem into a small set of compact equations, the geophysical community has been hesitant to move beyond *ad hoc* formulations. The directors method of *Mühlhaus et al.* [2004] is based on the theory of stratified composites. Although it seems to show interesting features for specific applications [*Lev and Hager*, 2008b], it does not really account for the underlying complex mechanical problem, i.e., the interaction between deforming grains. The kinematic model of *Ribe and Yu* [1991] (hereafter denoted "KR model") is based on a minimization of the strain-rate heterogeneity between grains (each grain is forced to deform as closely as possible to the polycrystal). It can be viewed as a relaxed version of the standard Taylor (uniform strain-rate) model that has been largely applied to cubic metals. However, the principle of minimum heterogeneity is known to provide a poor description of reality, although it leads at first order to LPO development that mimics laboratory constraints. *Kaminski et al.* [2004] further tentatively introduced grain boundary sliding (gbs) to obtain more reliable LPO evolution. But note that since there is no rheological parameter associated with gbs in this model, this mechanism is not taken into account as such. The main drawbacks of this formulation are the incorrect prediction that olivine polycrystals can deform with only three independent slip systems, and the impossibility of solving for the effective (anisotropic) viscosity at the polycrystal level, unless additional assumptions are introduced.

[7] Recrystallization is documented to have occurred in field samples exposed at the Earth's surface [*Ismail and Mainprice*, 1998] as well as in laboratory experiments [*Zhang et al.*, 2000], and it affects LPO development significantly. Although mechanisms active *in situ* and under laboratory conditions may be significantly different due to a huge difference in strain-rates (~10 orders of magnitude – this may have a large influence on the stored energy associated with dislocations storage), recrystallization has been tentatively introduced in micromechanical models, so far only in the KR [*Kaminski and Ribe*, 2001] and the TGT [*Wenk and Tomé*, 1999] models, with differences in these formulations that renders direct comparisons difficult. Both formulations are based on specific laws for nucleation, grain boundary migration, and stored energy distribution associated with dislocation densities.

3. Studied Case

[8] We consider velocity gradients that are predicted to occur along a mantle flow path beginning in the upwelling zone beneath an oceanic spreading center and ending several hundred kilometers away from the axis, driven by horizontal plate motion of 20 mm/yr, a typical slow spreading rate (Figure 1). We chose this streamline because it contains several aspects that a flow field near a plate boundary would contain, in particular rapid changes of deformation path: flow evolves from nearly vertical simple shear in the upwelling region, to significant axial straining around the flow corner, and ends with a nearly horizontal simple shear far from the spreading center. This corresponds to streamline #1832 of *Blackman et al.* [2002].

[9] We have used this velocity gradient as input of the aforementioned micromechanical models in order to compare their predictions in terms of LPO evolution along the flow path and the associated anisotropic rheological response (note that although a 2-D velocity gradient is considered, fully 3-D LPO calculations have been performed). For this, we assume that grains deform by dislocation glide on specific slip systems; the rheological behavior is given by a standard power law

$$\dot{\gamma}_{(k)} = \dot{\gamma}_0 \left| \frac{\tau_{(k)}}{\tau_{0(k)}} \right|^{n-1} \frac{\tau_{(k)}}{\tau_{0(k)}} \qquad (1)$$

with $\dot{\gamma}_{(k)}$ the rate of slip, $\tau_{(k)}$ the shear stress, and $\tau_{0(k)}$ the critical stress of system (k). We have adopted the classical value $n = 3.5$ for the stress sensitivity [*Durham et al.*, 1977; *Bai and Kohlstedt*, 1992]. We have considered the following slip systems (0 1 0)[1 00], (0 0 1)[1 0 0], and (0 1 0)[0 0 1], with respective critical stresses $15\tau_0$, $16\tau_0$, and $40\tau_0$ (τ_0 is an arbitrary reference stress). Therefore, *a* slip is easier than

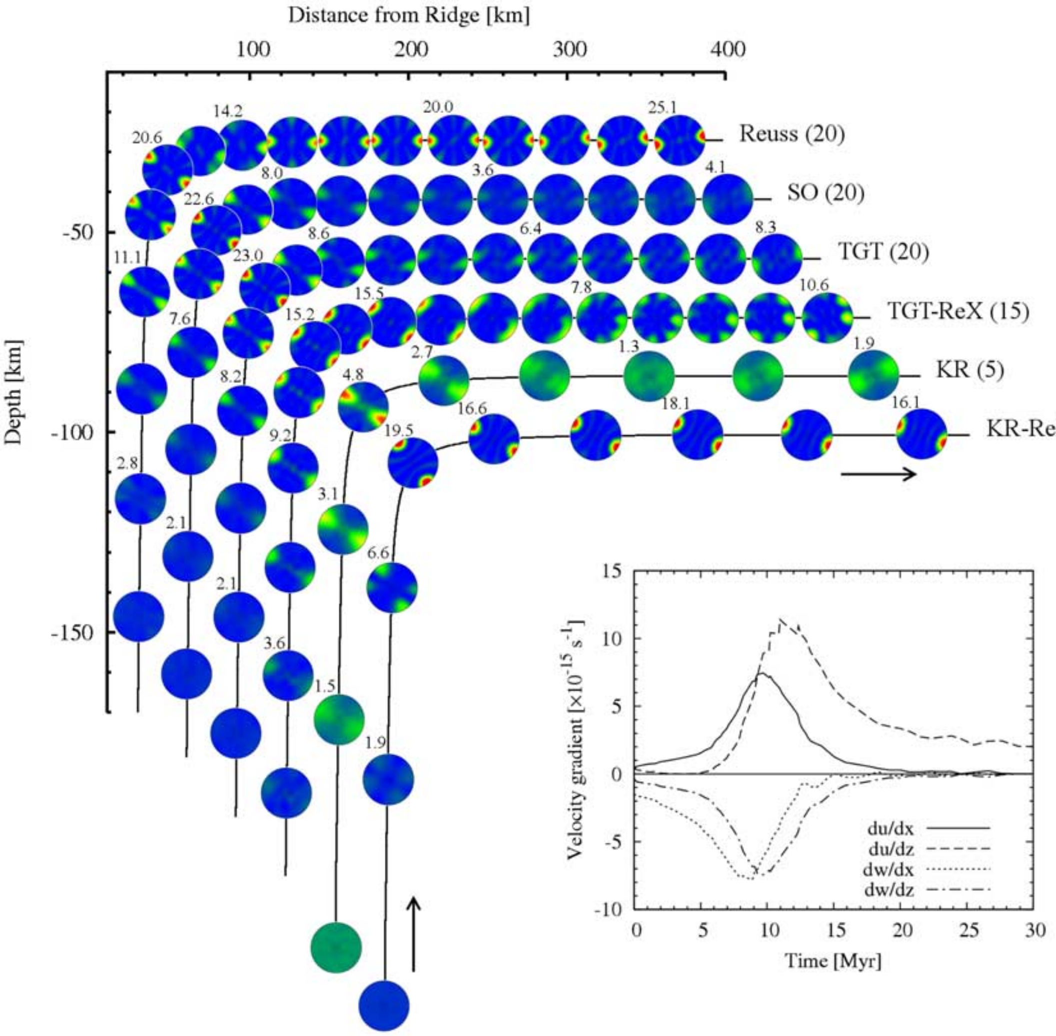

Figure 1. LPO predictions at different positions along streamline #1832, for Static (Reuss), SO, TGT (or VPSC), and Kinematic (KR) micromechanical models. Simulations including recrystallization effects are indicated with "ReX". (100) pole figures. The numbers above pole figures indicate their maximum intensity (relative to random LPO). Numbers in parentheses indicate the range used for the color scale. Inset: velocity gradient along the streamline, with x and z axes respectively horizontal and vertical, and u and w the corresponding velocities. With time origin taken at the streamline start (170 km depth), the flow corner is reached after ~12 Myr.

c slip, as expected for dry olivine crystals deformed under high temperature and low pressure.

[10] Since the SO model requires four independent slip systems, an additional system $\{10\bar{1}\}\langle 101\rangle$ must be introduced. This last system is not observed in natural olivine, but it is a simple (although not very accurate) way to mimic the possible effects of accommodation processes (e.g., simultaneous climb of a and c dislocations) that must be activated to allow olivine polycrystals to deform [*Castelnau et al.*, 2008b]. This system allows the crystal lattice to deform axially along a and c directions, but still not along b. Its resistance has been set to 100 times larger than that of (0 10)[1 0 0] so that its activation remains very small. For Reuss and TGT models, this system is not necessary nor would its inclusion influence the results.

[11] Finally, both TGT and KR models have been run with and without accounting for recrystallization processes. For simulations with recrystallization, we used parameters given in the original papers [*Wenk and Tomé*, 1999; *Kaminski et al.*, 2004], which were adjusted by these authors to match several experimental results under monotonic strain paths.

4. LPO Development

[12] Figure 1 shows LPO evolution along streamline #1832 obtained by the aforementioned micromechanical models when initially randomly oriented aggregates of olivine are subjected to the corresponding velocity gradient. Along the vertical path, and up to the flow corner, LPO development essentially consists of the progressive alignment of the a axis with the Finite Strain Ellipsoid (FSE). This feature is observed for all models tested here, including those for which recrystallization is included. The major difference between models concerns LPO strength, with significantly less pronounced texture for the KR model (without recrystallization) as compared to other models (in

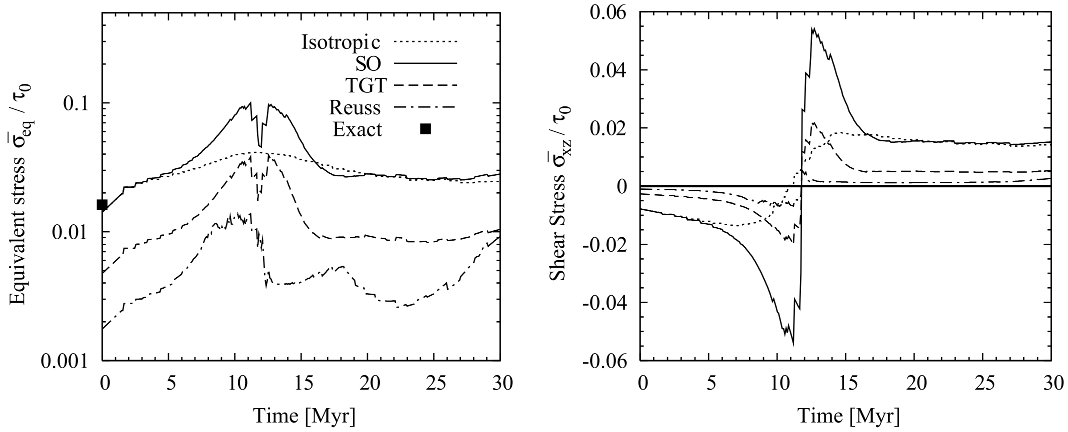

Figure 2. Evolution of (left) the equivalent stress $\bar{\sigma}_{eq} = \sqrt{3\bar{\sigma}_{ij}\bar{\sigma}_{ij}/2}$ and (right) the shear stress $\bar{\sigma}_{xz}$ along streamline #1832 as predicted by SO, TGT, and Reuss models. The black square corresponds to the "exact" flow stress (see text for details). Stress evolution in the isotropic case (i.e., keeping the LPO random along the whole streamline) is included for comparison.

Figure 1, the maximum intensity of pole figures provides a quantitative measurement of the LPO strength.). This observation is consistent with results obtained by *Kaminski and Ribe* [2001], and with the observation that LPOs obtained with the uniform strain-rate model (the solution that KR model tries to match as closely as possible) are generally less pronounced than those obtained with all other micromechanical models.

[13] After the flow corner where there is a rapid change in shear direction and shear sense, the LPO patterns vary significantly from one model to another. Basically, Reuss, KR, TGT, and SO models predict an alignment of [100] axes with the FSE, but the strength of LPOs are very different, from very sharp (Reuss) to almost random and probably too smooth (KR). The TGT model has been tested in the literature against numerous experimental results on metals, and it has been shown to provide accurate results except for the LPO strength which is generally too high – an effect attributed to intragranular strain heterogeneities not taken into account for LPO predictions [*Castelnau et al.*, 2006]. With respect to this, the smoother LPO predicted by the SO model can be considered as an improvement with respect to TGT.

[14] When recrystallization effects are accounted for, TGT and KR models simply predict different LPOs. The reason for such discrepancies is twofold. First, recrystallization is a poorly understood mechanism, even in standard metals. A universal theory to explain recrystallization has not been proposed so far, for any material. Even the most advanced recrystallization models are largely empirical and not really predictive although it is believed that they capture some of the physical mechanisms occurring in peridotites [*Piekos et al.*, 2008; *Wenk and Tomé*, 1999]. Secondly, the activation of recrystallization mechanisms strongly depends on the micromechanical model employed. For example, hard grain orientations are predicted to store more strain energy than the polycrystal average according to the uniform strain-rate (Taylor) model, but less than average according to the uniform stress (Reuss) model [*Bacroix et al.*, 1999]. Since this has strong influence on LPO patterns after recrystallization, we anticipate that the use of a more accurate micromechanical models (such as SO) is probably necessary to obtain reliable results.

5. Rheological Implications

[15] We now investigate the influence that LPO development may have on the rheology. Flow stress evolution along the flow path #1832 is shown in Figure 2. Results of the KR model are not presented since this model does not allow stress estimation.

[16] At the initial time $t = 0$ where orientations are random and rheology isotropic, very large stress differences are obtained between SO, TGT, and Reuss models. An "exact" result from *Castelnau et al.* [2008b], obtained with a numerical full-field technique, is given for comparison. As already pointed out, only the SO model provides the correct effective stress level (in the sense that the link between single crystal and polycrystal rheologies is correctly treated). In comparison, overall viscosities predicted by TGT and Reuss models are significantly underestimated.

[17] As strain (and time) increases, LPO development leads to an increasing stiffness of olivine as attested by the increase of the (absolute value of) shear stress, up to the flow corner at $t \simeq 12$ Myr. At the flow corner, shear changes sign quickly giving rise to a sudden drop of the equivalent stress, for a short time. Stress evolves qualitatively (but not quantitatively) similarly for SO and TGT models, but note that Reuss behaves significantly differently, next to the flow corner but also at the far end of the streamline (large *t*) where olivine is predicted to become stiffer again.

[18] For comparison, the SO model has been run with the same input data, but this time preventing LPO evolution (LPO thus remains random and olivine isotropic along the whole streamline). Large differences between isotropic and anisotropic cases are observed, and particularly in the region of the flow corner where stresses differ up to a factor $\sim$3. Since power law behavior is considered here, these differences roughly translate into a factor $3^{n-1} \simeq 15$ in the viscosity. It is also found that LPO-induced anisotropy leads to an even larger difference between directional viscosities for a given LPO, up to more than two orders of magnitude,

depending on the direction in which the olivine is deformed. We cannot address here the extent to which this local rheological effect will feedback into overall flow pattern. But based on results of previous studies showing (in an isotropic context) a strong feedback between the overall viscosity, melt production in the upwelling region, and strain localization [*Blackman et al.*, 1996, 2002], we anticipate that such order of magnitude variations are large enough to modify the flow strongly. Similar conclusions have been drawn by *Mangeney et al.* [1996] and *Mangeney and Califano* [1998] for the effect of LPO-induced anisotropy on the flow of ice in ice sheets (with a Reuss-type micromechanical model known to underestimate the rheological anisotropy), and recently by M. Knoll et al. (Multiscale modelling of the effect of preexisting lithospheric-scale wrench faults on the deformation of continental plates, submitted to *Geochemistry Geophysics Geosystems*, 2009) for the reactivation of inherited regions in the continental lithosphere.

[19] These results motivates our current work where explicit calculations of rheological feedbacks on flow evolution near plate boundaries will be fully assessed.

6. Conclusions

[20] This work suggests the following conclusions and remarks:

[21] 1. Compared to simple (monotonic) flow paths, the differences between LPO prediction models is enhanced when considering complex flow patterns.

[22] 2. The relation between single crystal and polycrystal rheologies is treated correctly only with the SO model so far. This model correctly requires four independent slip systems to allow olivine polycrystals to deform. This accuracy allows us to account for an improved physically-based rheology at the grain scale (such as temperature, pressure, and H_2O dependence of slip system strength) as described by *Cordier et al.* [2005], and to introduce (subtle) accommodation processes such as dislocation climb that in turn largely control the rheology.

[23] 3. The implementation of the SO model requires greater numerical effort than simpler approaches (e.g., it took about an hour on a standard workstation for a complete flow line calculation). This is probably unavoidable to get reliable predictions.

[24] 4. There is a crucial need to improve recrystallization models and to validate them for *in situ* conditions (extremely small strain-rates).

[25] 5. Rheological anisotropy associated with pronounced LPOs has a significant influence on the flow stress in regions of rapidly changing flow direction, with 1–2 orders of magnitude variation in directional viscosities compared to the isotropic case. Therefore, there is a potential for it to have a strong effect on *in situ* flow pattern.

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