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Effective viscoplastic behavior of polycrystalline aggregates lacking four independent slip systems inferred from homogenization methods; application to olivine

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ABSTRACT

Polycrystalline aggregates lacking four independent systems for the glide of dislocations can deform in a purely viscoplastic regime only if additional deformation mechanisms (such as grain boundary sliding and diffusion) are activated. We introduce an implementation of the self-consistent scheme in which this additional physical mechanism, considered as a stress relaxation mechanism, is represented by a nonlinear isotropic viscoplastic potential. Several nonlinear extensions of the self-consistent scheme, including the second-order method of Ponte-Castañeda, are used to provide an estimate of the effective viscoplastic behavior of such polycrystals. The implementation of the method includes an approximation of the isotropic potential to ensure convergence of the attractive fixed-point numerical algorithm. The method is then applied to olivine polycrystals, the main constituent of the Earth's upper mantle. Due to the extreme local anisotropy of the local constitutive behavior and the subsequent intraphase stress and strain-rate field heterogeneities, the second-order method is the only extension providing qualitative and quantitative accurate results. The effective viscosity is strongly dependent on the strength of the relaxation mechanism. For olivine, a linear viscous relaxation (e.g. diffusion) could be relevant; in that case, the polycrystal stress sensitivity is reduced compared to that of dislocation glide, and the most active slip system is not necessarily the one with the smallest reference stress due to stress concentrations. This study reveals the significant importance of the strength and stress sensitivity of the additional relaxation mechanism for the rheology and lattice preferred orientation in such highly anisotropic polycrystalline aggregates.

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Table 1
List of acronyms.

FFT	Fast Fourier transform
LPO	Lattice preferred orientation
SC	Self-consistent model
SEC	Secant estimate
TGT	Tangent estimate
AFF	Affine estimate
VAR	Variational estimate
SO	Second-order estimate
NPLCP	N-phase linear comparison polycrystal

1. Introduction

Physically based scale transition models are essential to establish the relation between the microstructure of polycrystalline aggregates and their effective viscoplastic properties. The accuracy of predictions is a key parameter to understand and model texture evolutions and the induced effective anisotropy. On the one hand, full-field approaches based on crystal plasticity have been proposed to compute the response of specific microstructures, using the Finite Element Method (see, e.g. Sarma and Dawson, 1996; Bhattacharya et al., 2001; Kanit et al., 2003) or Fast Fourier Transforms (FFT; acronyms used in this paper are listed in Table 1) (see, e.g. Moulinec and Suquet, 1998; Lebensohn, 2001). Despite the development of novel and very efficient methods such as FFT, the size of simulated representative volume is limited, and computations are CPU demanding. On the other hand, mean-field approaches such as those based on the self-consistent (SC) scheme, rely on a statistical description of the microstructure and are very powerful for the prediction of the effective behavior and the development of Lattice Preferred Orientation (LPO) at large overall strain. For nonlinear behavior, the main drawback is the necessary linearization of the local constitutive behavior that can critically affect the results consistency (see Ponte Castañeda and Suquet, 1998, for a review).

In this work, we will focus on the effective viscoplastic behavior of polycrystals lacking four independent slip systems. The vast majority of minerals constituting the Earth's mantle, such as olivine and pyroxenes, belongs to this class of materials (Karato, 2007). Similarly, many synthesized materials, such as semi-crystalline polymers (see, e.g. Bowden and Young, 1974; Argon, 1997; Seguela, 2007), do not exhibit four independent slip systems. It is worth noting that *five* independent slip systems are necessary to accommodate any arbitrary plastic strain at the local (i.e. grain) scale – this is the so-called von Mises criterion. However, SC estimations (Hutchinson, 1977; Nebozhyn et al., 2000) but also full-field computations (Castelnau et al., 2008a; Lebensohn et al., 2011) have shown that *four* independent systems are sufficient to ensure the polycrystal to deform as a whole, i.e. to guarantee a finite flow stress for any prescribed overall strain-rate.

The kinematic constraints induced by the lack of four independent slip systems lead to an indeterminacy of part of the deviatoric stress tensor. Only few attempts in the literature tried to address this issue. Parks and Ahzi (1990) proposed an ad hoc formulation, using Lagrange multipliers to determine unknown stress components, allowing the polycrystal to undergo viscoplastic strain with less than four independent slip systems. In the geophysical community, the purely kinematic model proposed by Ribe and Yu (1991), and extended by Kaminski and Ribe (2001) to include recrystallization effects, is widely spread and used; this relatively simple and intuitive formulation, which does not permit an estimation of the effective flow stress, also allows olivine polycrystals to deform with less than four independent slip systems, in qualitative contradiction with full-field results. Finally, a number of papers, e.g. Wenk et al. (1991), Tommasi et al. (1999, 2000), and Blackman et al. (2002) have applied the tangent (TGT) extension of the SC scheme (Lebensohn and Tomé, 1993) to olivine polycrystals; for purely numerical purpose, these authors introduced an artificial additional slip system with a large resistance to slip. It turns out that the TGT model incorrectly predicts a finite effective flow stress with only three independent slip systems (Castelnau et al., 2008a,b, 2010), a limitation that also affects microstructure evolutions at large strain (Castelnau et al., 2009).

Within the SC scheme, initially proposed for linear (e.g. thermo-elastic) polycrystals, all grains exhibiting the same crystal orientation are treated as a single (mechanical) phase. The SC scheme describes the statistical interaction between each phase and the surrounding polycrystal using the analytical solution of Eshelby (1957) to account for the interaction between an ellipsoidal inhomogeneity within a homogeneous linear matrix. The behavior of the surrounding polycrystal can then be obtained using the consistency conditions. Note that, at large strain, microstructure evolutions predicted by the SC scheme still suffer inconsistency due to an incomplete knowledge of the intragranular strain field, as illustrated in Castelnau et al. (2006) for the case of strain-hardening.

For nonlinear polycrystals, a linearization of the local constitutive behavior is necessary, leading to the definition of a N-Phase Linear Comparison Polycrystal (NPLCP). The standard thermo-elastic SC solution can then be applied to the NPLCP, from which the behavior of the original nonlinear polycrystal can be derived. This linearization step is not trivial, this is why several extensions of the SC scheme have been proposed in the literature, e.g. the secant (SEC)