Modeling the plastic deformation of olivine by dislocation dynamics simulations

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ABSTRACT

This work addresses the modeling of dislocation interactions and dynamics in olivine. A 3D dislocation dynamics (DD) simulation developed for cubic and hexagonal metals is adapted to the orthorhombic symmetry of this mineral. Dislocation core effects and mobilities are introduced through available models or phenomenological laws and fitted based on available experimental results on single crystals. The stress dependencies of the mobilities of [100] and [001] dislocations are emphasized. Dislocations interactions are studied through a simple elastic analysis and further using a more realistic approach based on DD simulations. It is shown that no junction formation results from the interaction between [100] and [001] dislocations. The collinear interaction is thus the only potential mechanism for forest hardening although its efficiency is significantly reduced by lattice friction on screw dislocations, which decreases the probability for dislocation reactions. The Taylor relationship is often used to model the dependence of the flow stress with the dislocation density. In the presence of a strong lattice friction, Taylor strengthening is shown here to be only a minor contribution to the flow stress and should not be responsible for it.

Keywords: Olivine, plastic deformation, simulation, dislocation dynamics

INTRODUCTION

Large-scale dynamic processes in the Earth, like mantle convection or subduction, involve plastic deformation of rocks and of their constitutive minerals. Over the last decades, several studies have established the role played by dislocation mechanisms in the creep flow of rocks and minerals. Thus, it appears necessary to develop a multi-scale modeling of the mechanical properties from atomic scale mechanisms in elementary minerals up to the macroscopic scale of rocks. One difficulty consists in accounting for the complex mechanisms of dislocation motion and interactions. This description is however crucial for Earth studies as laboratory data need to be transferred to very long time scales. The aim of the present work is to propose a first numerical model for the plastic deformation of olivine based on dislocation dynamics (DD) simulations.

In the past decade, the rapid increase in computing power has allowed developing 3D DD simulations in which the plastic deformation of a volume element is deduced from a physically based evolution of the dislocation microstructure. So far, this approach has been mainly applied to simple crystallographic structures like FCC metals (Kubin et al. 1992; Devincre and Kubin 1994; Madec et al. 2002a, 2003a), BCC metals (Tang et al. 1998, 1999), diamond-cubic structures (Moulin et al. 1997, 1999), or hexagonal metals (Monnet et al. 2004).

Olivine is widely considered to be the main constituent of the Earth’s upper mantle (down to a depth of 410 km) and to control the rheology of upper mantle assemblages. The structure of olivine is based on a distorted hexagonal close-packed oxygen sublattice. Olivine is orthorhombic with lattice parameters $a = 4.76$ Å, $b = 10.21$ Å, and $c = 5.98$ Å (Smyth and Hazen 1973). Numerous deformation experiments have been performed on olivine and forsterite single crystals (Kohlstedt and Goetze 1974; Durham and Goetze 1977; Durham et al. 1977, 1979; Darot and Gueguen 1981; Gueguen and Darot 1982) with a view to characterize the slip geometry. The main results can be summarized as follows. The most common dislocations have Burgers vectors $b$ that corresponds to the shortest lattice repeats [100] and [001]. The [010] dislocations are scarcely observed and do not seem to participate to plastic deformation in olivine. The [100] dislocation loops can glide on (010) planes where they exhibit long straight edge segments while the screw segments appear to be much shorter and curved. This general shape is confirmed by transmission electron microscopy (TEM) investigations (Durham et al. 1977; Gueguen and Darot 1982; Kashima et al. 1983). In (001) planes, gliding [100] loops are characterized by long straight screw segments (Durham et al. 1977). Above 1600 °C, edge segments appear to be short and curved. They disappear at 1150 °C and are replaced by straight mixed segments with preferential directions along <110>$. [100] dislocations can also glide on {011}, {021}, and {031}, however information about the microstructures on these planes is very scarce. Dislocations with [001] Burgers vectors glide on the following planes: (100),