European Mineralogical Conference
Vol. 1, EMC2012-27, 2012
European Mineralogical Conference 2012

Modelling dislocation and plasticity in MgO and $MgSiO_3$ perovskite under lower mantle conditions

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Magnesium silicate perovskite and ferropericlase are the main constituents of the mineral assemblage of the lower mantle. The plastic properties of these minerals is of primary importance to model deformation and flow which are responsible for mantle convection. Numerical modelling provides an alternative to deformation experiments to address the behaviour of materials under extreme (P,T) conditions.

In this study, we use a hierarchical multiscale model to investigate the effect of high pressure on the plastic properties of mantle phases. The first step corresponds to atomic scale calculations of dislocation core structures and associated Peierls stresses. It is done using either "cluster type" calculations (involving pair-wise potentials) or the Peierls Nabarro model based on ab initio calculations of generalized stacking fault energies. In a second step, we apply the kink-pair model to calculate dislocation velocities in the thermally activated regime governed by lattice friction. We can then derive the evolution of CRSS as a function of both pressure and temperature.

This approach has been first applied to MgO. In this oxide, high pressures have a profound effect on dislocation core structures and shear stresses. Under lower mantle pressures, MgO exhibit a change in dominant slip systems and is characterized by a strong lattice friction whatever the slip system. However, the influence of strain rate (taken into account in the model counteract this effect). The model is now applied to $MgSiO_3$ perovskite for which we present the first results of dislocation core modelling.