Poster Session | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[PO-C1]Poster Session 1

Symposium C

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-08]Pressure effects on dislocation core structures in Mg_2SiO_4 olivine: insights from atomic-scale modeling

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Olivine $(Mg,Fe)_2SiO_4$, a silicate with orthorhombic structure, is one of the most common minerals. As an abundant phase of the upper Earth mantle, its plastic properties strongly constrained the thermal convection of Earth mantle in its upper part. Plastic deformation of olivine involves two types of dislocation corresponding to the shortest Burgers vector [001] and [100]. At low temperature and high stress, [001] slip is supposed to be the most predominant slip system whereas at high temperature and low stress, [100] dislocations dominate. Over the last decades, a number of different slip systems have been thus identified in various domain of temperature, strain rate or pressure.

In this study, we revisit plasticity of this silicate by computing at the atomic scale the intrinsic properties of dislocation in Mg_2SiO_4 single crystal. All the calculations rely on a parametrized potential combining coulombic interactions and a core-shell interaction model for oxygen atoms. We performed a systematic investigation of [100] dislocations metastable configurations and possible dissociations.

Our calculations show that at low pressure, the atomic arrangement within the dislocation core is compatible with the [100](010) slip system observed experimentally. Also we show that the occurrence of several metastable core configurations allows to various cross slip events for which the cross slip energy barrier have been computed. Finally, we will show that the various core configurations are strongly sensitive to pressure leading to some change in the relative metastable states of the dislocation core and ultimately inhibiting some known slip plane at higher pressure.