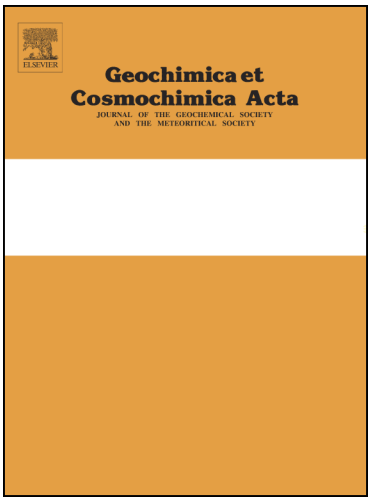

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PII: S0016-7037(17)30582-3
DOI: http://dx.doi.org/10.1016/j.gca.2017.09.026
Reference: GCA 10474

To appear in: *Geochimica et Cosmochimica Acta*

Received Date: 8 March 2017
Accepted Date: 12 September 2017

Please cite this article as: Mantisi, B., Sator, N., Guillot, B., Structure and transport at grain boundaries in polycrystalline olivine: an atomic-scale perspective, *Geochimica et Cosmochimica Acta* (2017), doi: http://dx.doi.org/10.1016/j.gca.2017.09.026

Structure and transport at grain boundaries in polycrystalline olivine: an atomic-scale perspective.

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ABSTRACT

Structure and transport properties at grain boundaries in polycrystalline olivine have been investigated at the atomic scale by molecular dynamics simulation (MD) using an empirical ionocovalent interaction potential. On the time scale of the simulation (a few tens of nanoseconds for a system size of ~650,000 atoms) grain boundaries and grain interior were identified by mapping the atomic displacements along the simulation run. In the investigated temperature range (1300 – 1700 K) the mean thickness of the grain boundary phase is evaluated between 0.5 and 2 nm, a value which depends on temperature and grain size. The structure of the grain boundary phase is found to be disordered (amorphous-like) and is different from the one exhibited by the supercooled liquid. The self-diffusion coefficients of major elements in the intergranular region range from ~ 10^{-13}-10^{-10} m^2/s between 1300 and 1700 K (with $D_{Si}^{gb} < D_{O}^{gb} < D_{Fe}^{gb} < D_{Mg}^{gb}$) and are only one order of magnitude smaller than those evaluated in the supercooled melt. In using a newly derived expression for the bulk self-diffusion coefficient it is concluded that the latter one is driven by the grain boundary contribution as long as the grain size is smaller than a centimeter. In assuming that the electrical conduction at grain boundaries is purely ionic, the macroscopic grain boundary conductivity is found to be two orders of magnitude lower than in molten olivine, and one order of magnitude higher than the lattice conductivity. A consequence is that the conductivity of the olivine polycrystal is dominated by the grain interior contribution as soon as the grain size is larger than a micrometer or so. The grain boundary viscosity has been evaluated from the Green-Kubo relation expressing the viscosity as function of the stress tensor time correlation function. In spite of a slow convergence of the calculation by MD, the grain boundary viscosity was estimated about ~10^5 Pa.s at 1500 K, a value in agreement with high-temperature viscoelastic relaxation data. An interesting information gained from MD is that sliding at grain boundaries is essentially controlled by the internal friction between the intergranular phase and the grain edges.

Keywords**:** Molecular dynamics simulations, classical force field, polycrystalline olivine, grain boundaries, pair distribution functions, self-diffusion coefficients, viscosity, electrical conductivity.