

## Grain boundary properties of polycrystalline olivine by molecular dynamics simulations

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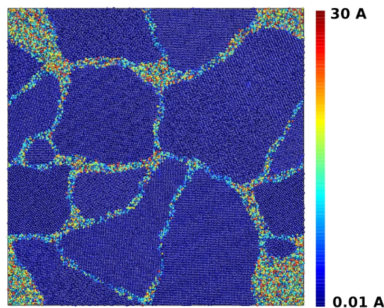
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Many properties of polycrystalline materials at high temperature and pressure are controlled by phenomena occurring at grain boundaries: incorporation and diffusion of incompatible elements, phase transitions, mechanical and transport properties... However several questions are still pending or remain controversial, because of the difficulty of determining experimentally at high temperature the grain boundary structure and the associated transport properties.

Here we propose an atomic-scale view of the structure and transport properties at grain boundaries in polycrystalline olivine, based on classical molecular dynamics simulations (over a few tens of nanoseconds for a system size of  $\sim 650,000$  atoms).

In the investigated temperature range (1300 - 1700 K) at 1 GPa, the mean thickness ( $\sim 1$  nm), the disordered microscopic structure of the grain boundary phase and the transport properties (diffusion, electrical conductivity and viscosity) of the polycrystal



Atomic displacement after 3ns  
in polycrystalline olivine at 1700K and 1GPa

are studied as a function of the grain size.

We find that in mantle olivine at depth, where grain size is in general smaller than a millimeter, the bulk diffusion of elements is mainly governed by grain boundary diffusion.

On the contrary, the contribution of the grain boundaries to the total conductivity of the polycrystal becomes negligible with respect to the grain interior conductivity, as soon as the grain size is greater than  $\sim 1 \mu\text{m}$ . Finally the grain boundary viscosity can be estimated and found to be essentially controlled by the slowest atoms of the grain boundary phase. The resulting viscosity value is several orders of magnitude higher than the one of the supercooled bulk melt.