Investigation of partial melting by atomistic simulation.

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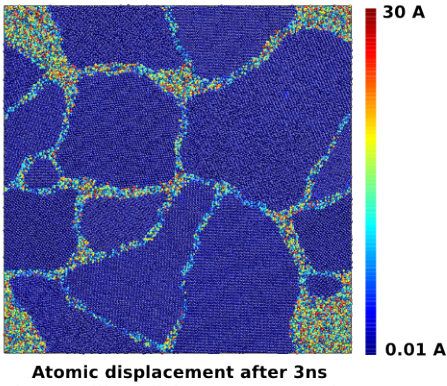
Partial melting plays a key role in the seismic and conductivity anomalies observed in the asthenosphere. Here we investigate by molecular dynamics simulation the transport properties of two model systems in partial melting, an ultrafine-grained olivine and a polycrystalline olivine (San Carlos) wetted by a MORB melt. The advantage of atomistic simulations is to provide a clear picture at the atomic scale of transport mechanisms acting in interphase boundaries. For the ultrafine-grained olivine (see the figure), we found that diffusion of elements through grain boundaries is several orders of magnitude greater that in the crystal structure. The activation energy of the electrical conductivity of the simulated system is in good agreement with the experimental data [1] although its magnitude is one order of magnitude too high, because of the small grain size investigated (~0.02 μ). More than 90% of the calculated conductivity is generated by the diffusion of Mg and Fe atoms within the grain boundaries the rest of it being generated by the slower diffusion of elements located in the first boundary layer of the grains. Moreover, the conductivity of the simulated olivine increases significantly with the Fe concentration, as observed experimentally [1]. With regard to the olivine-basalt system (2 wt% MORB), the calculated electrical conductivity is in agreement with experimental data [2] whereas the conductivity of the melt alone is evaluated and compared with that of the total system (Archie's law). The effect of the temperature, the pressure, the grain size, and the melt fraction is also discussed.



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

[1] Dai L. et al. (2014), *Phys Earth. Planet. Inter.* **237**, 73-79. [2] Yoshino T. et al. (2010), *Earth Planet. Sci. Lett.* **295**, 593-602