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Molecular Dynamics Simulations of Olivine-Silicate Melt Interfaces

Samia Gurmani (1,2), Sandro Jahn (1), Heinrich Brasse (2), and Frank R.Schilling (3)

(1) GFZ German Research Centre for Geosciences, Section 3.3, Telegrafenberg, 14473 Potsdam, Germany (samia@gfz-potsdam.de), (2) Freie Universität Berlin, Fachrichtung Geophysik, 12249 Berlin, Germany, (3) Institut für Bodenmechanik und Felsmechanik, Universität Karlsruhe, 76128 Karlsruhe, Germany

Partially molten rocks are important constituents of the Earth's crust and mantle. Their properties depend not only on the chemistry and mineralogy but also on the fraction and distribution of melt or fluid. Partially molten rocks strongly influence the chemical transport in the Earth and geodynamics. We model a partially molten rock on the atomic scale by confining a silicate melt of MgSiO3 composition between Mg2SiO4 olivine crystals. Molecular dynamics simulation is used to study the atomic scale structure and respective transport properties at the interfaces. To represent the atomic interaction, we use an advanced ionic model that accounts for anion polarization and shape deformations (Jahn and Madden, 2007). We construct interfaces between silicate melt layers of different thickness (1.85nm & 3.7nm) and mineral surfaces with different crystal orientations ((010), (001) and (100)). From the particle trajectories we derive various properties like charge density, cation coordination, connectivity of SiO4 tetrahedra and self diffusion coefficients. By adding some (Al, Ca) impurities to the system, the response to different chemical compositions is studied. To obtain a stable solid-melt interface, a temperature of 2000K is chosen. Simulations are performed at ambient pressure. We examine how the chemical composition and the self-diffusion coefficients vary across the interface. Our results indicate that with increase of surface energy, the self-diffusion coefficients of the various species decrease. This may be related to the stronger interaction of the crystal surface with the melt when the surface energy is high, which leads to more structured melt close to the interface. In conclusion, our simulations provide insight into the relation between atomic scale structure and transport properties in partially molten rocks.

References

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