

## Structure and properties of forsterite-MgSiO<sub>3</sub> liquid interface

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Knowledge about viscosities and permeability of partial molten rocks is important to understand the thermal history of the Earth and volcanism. For understanding those obtained by experiments and estimating the physical properties at extreme conditions that difficult to reproduce in laboratory experiments, knowledge about structure and properties of silicate crystal-liquid interfaces is necessary. In this study, structure and properties of the forsterite-MgSiO<sub>3</sub> liquid interface are investigated by using molecular dynamics simulations. It is essential to know the structure and physical properties of forsterite-MgSiO<sub>3</sub> liquid interfaces since forsterite is the liquidus mineral of primordial magmas.

Molecular dynamics simulations were performed with NPT ensemble using MXDORTO code. The interatomic potential model used in this study is same with used in Noritake et al. (2012). The initial structure is 21440 atom system in which a sheet of MgSiO<sub>3</sub> liquid consist of 8000 atoms is sandwiched between (010) surfaces of forsterite and 43440 atom system in which a sheet of MgSiO<sub>3</sub> liquid consist of 30000 atoms is sandwiched between (010) surfaces of forsterite. Structure and properties in the vicinity of interface was obtained at 0.1 MPa and various temperatures.

From simulation results, characteristic structure was observed in the forsterite-MgSiO<sub>3</sub> liquid interface. In the crystal-liquid interface, 2-30% of SiO<sub>4</sub> tetrahedra of forsterite surface bridge SiO<sub>4</sub> tetrahedra in liquid. In liquid region, SiO<sub>4</sub> tetrahedra concentrate in the vicinity of surface and form an SiO<sub>4</sub> tetrahedra rich layer of 0.4 to 0.6 nm thickness. Inner side of the first SiO<sub>4</sub> rich layer in MgSiO<sub>3</sub> sheet in liquid, the Mg rich second layer of 0.6 nm thickness is formed. Consequently, the structure of liquid is different from that of bulk liquid in 1.2 nm from crystal-liquid surface. However, the biased concentration approaches to bulk composition with the distance from the interface. In the first layer, internal energy of the system is lowered by bridging between SiO<sub>4</sub> tetrahedra at the crystal-liquid interface, and Coulombic interaction between non-bridging oxygen in liquid and magnesium at the crystal surface. In the second layer, interaction between concentrated magnesium and excess oxygen by bridging lower the internal energy.

The 2D self-diffusion coefficient oxygen in the plane in first layer is a half order lower than that of bulk liquid. However, The 2D self-diffusion coefficient of oxygen in Mg-rich second layer is a half order higher than that of bulk liquid. Existence of bridging oxygen between crystal and liquid, and concentration of SiO<sub>4</sub> tetrahedra in first layer might decrease the self-diffusion coefficient of oxygen in the first layer. Concentration of free oxygen, non-bridging oxygen and magnesium might increase the self-diffusion coefficient of oxygen in second layer.

This simulation results suggest that existence of small amount of melt might considerably decrease the viscosities of partial molten rocks and considerably increase permeability of partial molten rocks. However, it should be confirmed that this double layered structure in forsterite-MgSiO<sub>3</sub> liquid interface is equilibrium by performing of long time calculations.

Keywords: Interface, Molecular dynamics simulation, Silicates, Crystal, Liquid