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Molecular dynamics simulations of sodium silicate melts

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Inter-atomic potentials are essential for precise reproduction and prediction of physical property of the system using molecular dynamics simulation. In the silicate system, many pair potential models have been proposed. Some of these can reproduce crystal structures and its elastic properties (e.g. van Beest et al. 1990) and were used for silicate melts (Lacks et al. 2005). However, these previous models which can reproduce qualitative pressure dependence of viscosity seem not to reproduce temperature dependence of Q-species (Maehara et al. 2005).Understanding the physical properties and their characteristic behavior of silicate melts, nano-structure and its temperature, pressure and composition dependence are needed to know.

To investigate the nano-structure of silicate melts, we employed newly developed inter-atomic potential model for silicate systems. Our potential model definitely includes coulombic interaction, short range repulsion, van der Waals interaction and radial covalent interaction terms. Molecular dynamics simulations were performed for $Na_2Si_2O_5$ system using the MXDORTO. The number of atoms, pressure and temperature are maintained constant (NPT ensemble, Natom=5994, P=0.1MPa). Physical property and Q-species were obtained at every 300K during the cooling from 3000K. The equilibrium data were obtained after 2-3ns (2-3,000,000steps) relaxation at each temperature. From this simulation, thermal expansion and temperature dependence of Q-species were investigated. The temperature dependence of Q-species was qualitatively reproduced, however it was not enough yet at quantative aspect.

To improve the inter-atomic potential parameters, we are performing MO calculation using Gaussian09. To focus on Si-O-Si bond, we calculated energy surfaces of silicate clusters contain Si-O-Si bond (e.g. dimer, rings) for structural changes. By fitting inter-atomic potential parameters to these energy surfaces, improvement of reproducibility of physical properties is expected and the relation between physical properties and atomic structure might be discussed.

Keywords: MD, molecular dynamics, silicate melt