Japan Geoscience Union Meeting 2014
(28 April - 02 May 2014 at Pacifico YOKOHAMA, Kanagawa, Japan)

SMP47-01 Room:422 Time:May 1 09:00-09:15

First-principles calculations of the structure of MgSiO3 melt at high temperature and high pressure

MATSUI, Masanori[1*]

[1]School of Sci., Univ. of Hyogo

Crystals and melts with MgSiO3 composition are important constituents of the Earth's lower crust and mantle. Therefore an accurate knowledge of their structural and elastic properties at high temperatures and high pressures is crucial to investigate the chemical and physical structures, and the conditions of formation and evolution of the Earth. However, reliable experimental data under geophysically relevant conditions are generally lacking for MgSiO3 melt, mainly due to the difficulty in obtaining such data at the combined high temperature and high pressure found in the Earth's interior. Here we use the first-principles molecular dynamics (FPMD) method to study the structures and elastic properties of MgSiO3 melt at high temperatures and high pressures.

All calculations were performed with the Vienna Ab Initio Simulation Package VASP (Kresse and Furthmuller, 1996). The projector-augmented wave (PAW) method was used in the local density approximation (LDA) for the exchange-correlation functional (Blochl, 1994; Kresse and Joubert, 1999). FPMD calculations were carried out in the canonical ensemble (constant temperature T, constant volume V, and constant number of atoms N in the system) using cubic basic cells. N was taken to be 160 (32 MgSiO3) throughout this study. After annealing the system sufficiently at 4000 K, and then 3000 K, we fixed V at 38.54 cm3/mol and T at 2000 K to calculate the interference function S(Q), where Q is the length of scattering vector, and the radial distribution function (RDF) for each atom pair. We found FPMD calculated S(Q) compares reasonably well with the observed data from X-ray analyses at 1973 K by Waseda and Toguri(1990). The FPMD predicted average nearest neighbor bond distances r(ij), and coordination numbers n(ij) between atoms i and j are also compared well with the data by Waseda and Toguri(1990), except the r(MgO) distance, in which the FPMD value of 1.97 A is much shorter than the value [2.12(1) A] by the X-ray analyses. We further apply the FPMD technique to investigate the temperature and pressure dependencies of the structure of MgSiO3 melt.

Keywords: MgSiO3 melt, high temperature, high pressure, first-principles calculation