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

SIT39-05 Room:416 Time:May 2 10:00-10:15

Small shear modulus of cubic CaSiO3 perovskite

KAWAI, Kenji[1*] ; TSUCHIYA, Taku[2]

[1]Department of Earth and Planetary Sciences, Tokyo Institute of Technology, [2]Geodynamics Research Center, Ehime University

Ca-perovskite (CaPv) is considered to be one of the most abundant minerals in the Earth's lower mantle (LM) and was suggested to have distinctly larger shear modulus than MgPv from static calculations and mean-field theory (Karki and Stixrude 1999; Stixrude et al. 2007). In this study the elasticity of cubic CaPv is reinvestigated using density functional constant-temperature first principles molecular dynamics simulations with strict calculation conditions. First, we computed the stable structure of CaPv and found that the cubic phase is more stable than the tetragonal and orthorhombic in the LM P,T condition. The thermal equation of state of CaPv was analyzed using the MD data set, which indicates its thermal properties including Gruneisen parameter quite similar to those of MgPv. Along the adiabatic temperature, CaPv was found to have higher density than the PREM and 12.5% iron-bearing MgPv. Next, we calculated elastic constants of cubic CaPv. Our new results clearly demonstrate that cubic CaPv does not have anomalously large shear modulus suggested by previous calculations with a small computation cell. This is because the cell applied in the previous studies is too small to allow the rotational phonon motion of SiO6 octahedra related to the zone boundary optic phonon instability. Acoustic wave velocities were finally determined from the elastic moduli, indicating no significant differences in velocities between CaPv and iron-bearing MgPv.

Keywords: Ca-perovskite, elasticity, lower mantle, first principles