Japan Geoscience Union Meeting 2013
(May 19-24 2013 at Makuhari, Chiba, Japan)

SMP44-P02 Room:Convention Hall Time:May 20 18:15-19:30

Volume and crystal structure change due to He incorporation into cristobalite at high pressures

Masanori Matsui[1*], Tomoko Sato[2], Nobumasa Funamori[3]

[1]School of Sci., Univ. of Hyogo, [2]Dept. of Earth and Planetary Systems Sci., Hiroshima Univ., [3]Dept. of Earth and Planetary Sci., Univ. of Tokyo

Based on powder X-ray diffraction measurements under high pressures and room temperature at Photon Factory, Tsukuba, Sato et al.(2012) have recently found unique behavior of cristibalite in helium pressure medium in a diamond anvil cell, where, on compression, cristobalite II transformes to a new phase (called cristobalite-He I) at about 8 GPa, then on subsequent decompression from about 15 GPa, cristobalite-He I transforms to another new phase (called cristobalite-He II) at about 7 GPa. They tentatively assigned cristobalite-He I and II to have orthorhombic and rhombohedral lattices with molar volumes greater than about 30 % and 25 % larger than cristobalite, respectively. Here we use first-principle calculations to study structural and enegetic properties of cristobalite-He I and II in more detail.

All calculations were performed with the ab initio simulation package VASP (Kresse and Furthmuller, 1996). The projector-augmented wave (PAW) method (Blochl, 1994) was used in the generalized-gradient approximation (GGA) for the exchange-correlation functional (Perdew et al., 1996). Atomic positions were relaxed with observed or hypothetical crystal-symmetry constraints. In order to check the reliability and applicability of the computations, we first calculated the structures and energies of cristobalite and cristobalite II, with the results that the calculated values reproduce the observed ones (Dove et al., 2000; Dera et al., 2011) accurately.

Cristobalite transforms to cristobalite II at 1.5 GPa and room temperature (Palmer and Finger, 1994; Dove et al., 2000). The initial lattice parameters and atomic positions of both Si and O were taken from cristobalite II (Dove et al., 2000; Dera et al., 2011), while the He positions were taken to be situated in large voids in cristobalite II. We tested several structural models for both cristobalite-He I and II, and finally found enthaly-minimized models that reproduces the measured X-ray diffraction patterns of the two phases (Sato et al., 2011), respectively, accurately.

Keywords: cristobalite, helium, high pressure, crystal structure, phase transition