Japan Geoscience Union Meeting 2015
(May 24th - 28th at Makuhari, Chiba, Japan)

SIT03-18 Room:106 Time:May 26 09:45-10:00

Post-perovskite phase boundary of Fe- and Al-bearing MgSiO3

WANG, Xianlong[1*] ; TSUCHIYA, Taku[1]

[1]GRC, Ehime University; ELSI, Tokyo Institute of Technology

The post-perovskite (PPv) phase transition of $MgSiO_3$ bridgmanite (Br) [1,2,3] occurs in the pressure (P) and temperature (T) conditions corresponding to the Earth's D? layer. Therefore, $MgSiO_3$ PPv is believed to be a key mineral to understanding the seismological properties in this layer. However, to date, it is still a challenging subject to determine the phase transition boundary preciously in the geophysically relevant Fe and Al-bearing compositions. Based on the first-principles methods combined with the internally consistent LSDA+U method and the lattice dynamics approach, the high-P and high-T thermodynamics of the $MgSiO_3$ phases are directly calculated with incorporation of 6.25 mol% of Fe^{2+}, $Fe^{3+}Fe^{3+}$, $Fe^{3+}Al^{3+}$, and $Al^{3+}Al^{3+}$ [4,5]. Using calculated free energies, we determine the PPv phase boundaries for Fe and Al-bearing compositions. Our results show that at 2500 K, the $Fe^{3+}Al^{3+}$ and $Fe^{3+}Fe^{3+}$ incorporations span coexisting domains between Br and PPv significantly with lowering the transition pressure, in contrast to the Fe^{2+}- and $Al^{3+}Al^{3+}$-bearing cases.

References:
[1] M. Murakami, K. Hirose, K. Kawamura, N. Sata, and Y. Ohishi, Science **304**, 855 (2004).
[2] A. Oganov, and S. Ono, Nature **430**, 445 (2004).
[3] T. Tsuchiya, J. Tsuchiya, K. Umemoto, and R. M. Wentzcovitch, Earth. Planet. Sci. Lett. **224**, 241 (2004).
[4] J. Tsuchiya, and T. Tsuchiya, Proc. Natl. Acad. Sci. USA **105**, 19160 (2008).
[5] A. Metsue, and T. Tsuchiya, Geophys. J. Int. **190**, 310 (2012).

Keywords: First-principles method, internally consistent LSDA+U, post-perovskite, phase transition