Effects of Fe and Al incorporations on $MgSiO_3$ postperovskite phase boundary

*Xianlong Wang[1,2], Taku Tsuchiya[3,4], Zhi Zeng[1,2]

1. Institute of Solid State Physics, Chinese Academy of Sciences, 2. University of Science and Technology of China, 3. Geodynamics Research Center, Ehime University, 4. Earth-Life Science Institute, Tokyo Institute of Technology

$MgSiO_3$ bridgmanite (Br) will undergoes a post-perovskite (PPv) phase transition[1,2,3] in the pressure (*P*) and temperature (*T*) conditions corresponding to the Earth's D" layer. Therefore, The phase change is recognized as the key for understanding the seismological observations in the D" 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,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, incorporations of $Fe^{3+}Fe^{3+}$ and $Fe^{3+}Al^{3+}$ 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, MgSiO3, postperovskite

