Implication of the B1-B2 phase transition on MgO diffusion properties in super-Earth mantles

*Sebastian Ritterbex¹, Takafumi Harada¹, Taku Tsuchiya¹

1. Geodynamics Research Center Ehime University

The mantle of the Earth and those of terrestrial exoplanets (super-Earths) is expected to be composed of high-pressure silicates and the oxide ferropericlase. Because the latter is considered to be weakest, the rheological properties of MgO periclase are thought to influence the dynamics and evolution of terrestrial planets. B1-type (Fm-3m) MgO is stable over the pressure range of the Earth’s mantle, but if pressure exceeds ~500 GPa in the mantle of super-Earths, B1-type MgO transforms into its B2-type (Pm-3m). Based on early results from analogue materials, Karato (2011) suggested that this B1-B2 MgO phase transition may affect mantle rheology by a viscosity decrease in super-Earths as opposed to the general trend expected of a viscosity increase with increasing depth.

To test the above hypothesis, we investigated self-diffusion in B2-type MgO via the vacancy mechanism by using first-principles calculations (Ritterbex et al. 2017). We elucidate that non-interacting vacancy pairs are most abundant in both the intrinsic and extrinsic regimes which may govern ionic diffusion. Across the phase transition, we find substantial reductions in defect energetics and show that the reduction in ionic migration enthalpy accounts for an increase in the effective MgO diffusion coefficient of ~10⁴ at 500 GPa. Our examination of atomic relaxations demonstrates that diffusion controlled viscosity may generally decrease across high-pressure phase transitions with increasing coordination number. Our results suggest mantle convection in the deep interior of super-Earths to be more vigorous than previously thought.

Keywords: super-Earths, B2-type MgO, diffusion properties