The 457th Geodynamics Seminar

Lattice diffusion in B2-type MgO

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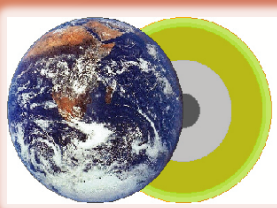

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Abstract

High-pressure and high-temperature rheology is important for understanding the dynamics of planetary interiors. Since the discovery of super-Earths, study has been conducted on its mantle convection. However, the rheological properties of constituent minerals under ultra-high-pressure have not been elucidated. In the super-Earths' mantle, diffusion creep might be one of the dominant viscoplastic mechanisms (e.g., Karato, 2011). Thus lattice diffusion coefficient (D) is a key property for understanding the mantle convection. Experimental measurements of D however still remain difficult under deep planetary conditions. Theoretical study is therefore currently a unique way at multi-megabar pressure.

B2 (CsCl)-type MgO is a high-pressure phase of B1 (NaCl)-type MgO and expected to be one of the major constituents in super-Earths' mantle (Schaefer and Fegley, 2009; Valencia *et al.*, 2010). A one-dimensional parameterized convection model with viscosity extrapolated by assuming constant activation volume of bridgmanite shows that CMB-lids develop (Stamenkovic *et al.*, 2012). However, Karato (2011) suggested that viscosity could decrease associated with the B1-B2 transition of MgO based on measured plasticity of analog materials. D of actual B2-type MgO is still underdetermined.

In my last GD seminar last year, I reported the calculated pressure dependence of migration enthalpy (H_m) of B1- and B2-type MgO, which is one of the key parameter to obtain D. In this seminar, I will talk about attempt frequency (ν), which is also another important parameter and is extracted from D near the melting P-T condition by first principles constant-temperature molecular dynamics method. I find that ν hardly changes across the B1-B2 transition. Finally, D is evaluated from H_m and ν. I identify distinctly D of both Mg and O in B2-type is larger than in B1-type at the same pressure. It suggests that B2-type would be less viscous as expected in Karato (2011). Additionally, the activation volume of B2-type MgO is lower than the value assumed by Stamenkovic *et al.* (2012). Super-Earths' mantle is expected to convect..

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