

The 431st Geodynamics Seminar

Migration enthalpy and lattice diffusion in B2-type MgO

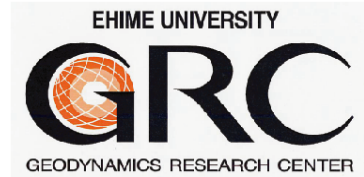
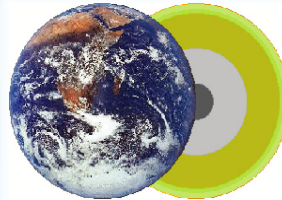
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Abstract

A high pressure and high temperature rheology of materials or minerals is important for understanding the dynamics in planets. The diffusion creep might be one of the dominant deformation mechanisms. Lattice diffusion coefficient D is a key property in this deformation process. Experimental measurements of D however still remain technically difficult under deep planetary conditions. Theoretical approaches therefore play a substantial role.

B2 (CsCl)-type MgO is a high pressure phase of B1 (NaCl)-type MgO. It is also expected one of the major minerals in super-Earths' mantle and giant planetary core. The previous study (Karato, 2011) suggested that diffusion creep viscosity of the super-Earths' mantles could decrease under ultra-high pressure due to the B1-B2 transition of MgO. However, his idea is based on measured plasticity of analog materials and diffusion coefficients of B2-type MgO themselves still remain unclear.

In our study, we calculate the migration enthalpy in B1- and B2-type MgO based on the first principles calculation in order to identify contrast in the diffusivity of B1 and B2 phase. Results indicate first that migration enthalpies of both Mg and O are smaller in B2-type than in B1-type as the same pressure, suggesting that B2-type would be less viscous. In addition, in B1-type the migration enthalpy of Mg is found to be smaller than that of O, while in B2-type the migration enthalpy of Mg is found bigger. In this talk, the mechanism of reduction in migration enthalpy will be discussed.