Lattice diffusion in B2-type MgO

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High-pressure and high-temperature rheology is essential for understanding the dynamics in planets. Diffusion creep might be one of the dominant viscoplastic mechanisms and lattice diffusion coefficient *D* is a key property in this deformation process (e.g., Karato, 2011). 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 and expected to be one of the major constituents in super-Earths' mantle and giant planetary core (Guillot, 1999; Tsuchiya and Tsuchiya, 2011). Although diffusion creep viscosity of super Earths' mantle is usually assumed to increase with depth monotonically, a previous study (Karato, 2011) suggested that it could decrease associated with the B1-B2 transition of MgO. However, this idea is obtained based on measured plasticity of analog materials and thus *D* of actual B2-type MgO is still underdetermined.
In this study, we calculate *D* of B1- and B2-type MgO based on first principles constant-temperature molecular dynamics method combined with static lattice energy calculations. We identify distinctly larger *D* of both Mg and O in B2-type than in B1-type at the same pressure, suggesting that B2-type would be less viscous as expected. The mechanisms of increase in *D* will be presented.

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