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MgO 格子原子拡散挙動の第一原理シミュレーション
Lattice diffusion in MgO crystal from first principles simulation

原田 隆史 [1*] ; 土屋 卓久 [1]
HARADA, Takafumi[1*] ; TSUCHIYA, Taku[1]

[1] 愛媛大学地球深部ダイナミクス研究センター
[1]Geodynamics Research Center, Ehime University

Rheological property is critical to understanding the mantle convection. Diffusion creep might be the dominant deformation mechanism in the Earth's lower mantle and super-Earths' mantle (e.g., Karato, 2011). Thus several experimental and theoretical studies have tried to measure lattice diffusion coefficients under pressure, which are both still technically difficult. There are two theoretical approaches to calculate self-diffusion coefficient in solids. One is based on the static lattice energy calculation and the other is based on the molecular dynamics simulation. In the former case, it is difficult to evaluate attempt frequency and in the latter case, atoms are hardly mobile in actual computation time at the Earth's lower mantle and super-Earths' mantle temperatures. These two approaches were previously applied to MgO, one of major deep mantle constituents (Ita & Cohen, 1997; Ito & Toriumi, 2007). However reported pressure dependences of the self-diffusion coefficients are contradictive with each other particularly at high pressure over 80 GPa.

In this study, we develop a new theoretical method to calculate self-diffusion coefficient in crystals with charged vacancies (Schottky pair) within the first principles framework. This method was then applied to NaCl-type MgO. We found that the calculated pressure dependences of the self-diffusion coefficients in MgO are consistent with those of Ita & Cohen (1997). Diffusion creep viscosity of MgO was then estimated using calculated diffusion coefficients. Our activation volumes are consistent with experimental values at low pressure (Van Orman et al., 2003) and decrease rapidly with increasing pressure. It suggests that super-Earths' mantle would not be quite viscous and the constant activation volume extrapolation leads to overestimation of viscosity in the deep mantle.

This method is widely applicable to other materials including bridgmanite, post-perovskite and CsCl-type MgO, which are important to analyze more realistic planetary interior dynamics.

キーワード: MgO, 格子拡散, 地球下部マントル, スーパーアースマントル, 第一原理計算
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