First-principles study on the site occupancy of Fe^{3+} in ferropericlase (Mg,Fe)O

*Hokai Fujitani[1], Taku Tsuchiya[1]

1. Ehime University Geodynamics Research Center

A high vacancy concentration due to the extrinsic mechanism is considered to be reproduced rheological property of Earth’s lower mantle via diffusion creep (e.g., Ita and Cohen 1998). Charge unneutral Fe^{3+} is one of the major impurities to create vacancies as the following reaction $3Mg^{\times} \rightarrow 2Fe^{\cdot} + V^{''}$. It has been experimentally reported that the site occupancy of Fe^{3+} changes from the octahedral site to the tetrahedral in MgO with increasing pressure around 15 GPa (Otsuka et al., 2010), leading to a further increase of the vacancy concentration in the octahedral site. However, little is known about the effects of Fe^{3+}/vacancy configuration and the spin transition on its site preference, the differences in chemical bonds around octahedral and tetrahedral Fe^{3+}. In this study, we investigate Fe^{3+} bearing MgO by using first-principles calculation methods based on the density functional theory up to 150 GPa. The tetrahedral occupation of Fe^{3+} is so fur not found in all the defect configurations and pressure condition examined, being not consistent with experimental findings.

Keywords: Fe3+, ferropericlase, First-principles calculation

