

The 401th Geodynamics Seminar

Solid solution effect of Fe^{2+} and Fe^{3+} on the elastic property of MgSiO_3 bridgmanite: an internally consistent LSDA+ U study

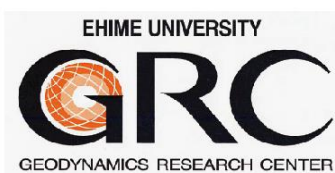
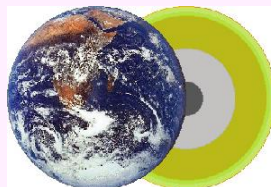
Atsushi Hase (Msc. Student, Ehime University)

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Abstract

Determination of the chemical composition of the Earth's lower mantle (LM) has long been a challenging subject in the deep Earth science. Reproduction of the seismological observations based on the elastic properties of dominated LM minerals is a powerful way to construct the reasonable LM composition model. However, experimental studies about solid solution effects of Fe^{2+} and Fe^{3+} on the elastic properties of MgSiO_3 bridgmanite (Br) at high-pressure and high-temperature are scarcity

On the other hand, our group had reported the solid solution effects of iron and aluminum on the elastic properties of Br relying on the first-principles calculations [Tsuchiya and Tsuchiya, 2006]. Nevertheless, since the computational resource is limited at that time, the study had some insufficient treatments as follows (i) Only the solid solution effects of Fe^{2+} were investigated, but Fe^{3+} did not. (ii) The exchange-correlation functional was described within GGA, which cannot sufficiently describe the large on-site Coulomb interactions among the 3d electrons in Fe-O bonds [Cococcioni and de Gironcoli, 2005]. Furthermore, GGA overestimates the volume of Br. (iii) The solid solution effects of Fe^{2+} on Br were estimated based on the properties of the end-member, FeSiO_3 -Br.

In this study, I calculate the solid solution effects of both Fe^{2+} and Fe^{3+} on the elastic properties of Br based on the first-principles calculations combined with the LSDA+ U exchange-correlation functional, which can correctly describe the large on-site Coulomb interactions among the 3d electrons in Fe-O bonds. The U values are obtained non-empirically based on the linear response theory [Cococcioni and de Gironcoli, 2005]. The Fe-bearing Br supercells with a 6.25 mol% of FeSiO_3 , Fe_2O_3 , and FeAlO_3 are used.

Our results show that Fe^{2+} and Fe^{3+} have different solid solution effects on the elastic properties of Br. Depending on the experimental report from Chantel et al. [Chantel et al., 2012], $(\text{Mg}_{0.95}\text{Fe}^{2+}_{0.04}\text{Fe}^{3+}_{0.01})\text{SiO}_3$ has values located between the simulated results of Fe^{2+} -bearing Br and Fe^{3+} -bearing Br, since they measured the effects of Fe^{2+} and Fe^{3+} together. This indicates that our theoretical studies and experimental observations of Chantel et al are harmonic.