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

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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], $(Mg0.95Fe^{2+}0.04Fe^{3+}0.01)SiO_3$ 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.

詳細は当センターホームページ：http://www.ehime-u.ac.jp/~grc/をご覧ください
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