The 426th Geodynamics Seminar

Solid solution effects of Fe2+ and Fe3+ on the thermo-elastic property of MgSiO3 bridgmanite calculated based on the internally consistent LSDA+U method

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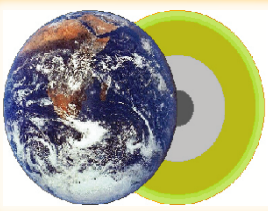

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Abstract

Determination of the chemical composition of Earth's mantle was a long-standing challenge in Earth science. A powerful way to build the composition model of lower mantle is to reproduce the seismological properties from the elastic properties of main material of lower mantle. Recently, our group reported that composition of the lower mantle is pyrolytic by the thermo-elastic properties based on the first-principles calculations [Wang et al (2015)]. In this study, I am going to report those solid solution effects of Fe^{2+} and Fe^{3+} on the elastic property of $MgSiO_3$ bridgmanite (Br) obtained Wang et al (2015). Local density approximation (LDA) and generalized gradient approximation (GGA) cannot reproduce the Fe-O bands correctly. Therefore, as with our calculation of the iron-containing Br, I calculate the thermo-elastic property of Fe-bearing Br based on the internally consistent LSDA+U method.

Result show that solid solution effects of Fe^{2+} and Fe^{3+} on the thermo-elastic property of Mg-Br are different value at 0~180GPa and 0~4000K.

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