Japan Geoscience Union Meeting 2014
(28 April - 02 May 2014 at Pacifico YOKOHAMA, Kanagawa, Japan)

SMP47-P01 会場:3 階ポスター会場 時間:5 月 1 日 18:15-19:30

Thermodynamic properties of Mg-postperovskite with Fe^{3+} and Al^{3+} dopant: an internally consistent LSDA+U study

Thermodynamic properties of Mg-postperovskite with Fe^{3+} and Al^{3+} dopant: an internally consistent LSDA+U study

WANG, Xianlong[1*] ; TSUCHIYA, Taku[1]
WANG, Xianlong[1*] ; TSUCHIYA, Taku[1]

[1]GRC, Ehime University and ELSI, Tokyo Institute of Technology
[1]GRC, Ehime University and ELSI, Tokyo Institute of Technology

Thermodynamic properties of $MgSiO_3$ perovskite (Pv) and postperovskite (PPv) with Fe and Al incorporation at high pressure and high temperature are important to understand the Earth's lower mantle (LM). The thermodynamic properties of Fe^{2+}, Fe^{3+}, and Al^{3+}-bearing Pv[1,2,3] and Fe^{2+}-bearing PPv[4] have been investigated in our previous works uniformally based on first-principles method combined with the internally consistent LSDA+U method and quasi-harmonic approximation (QHA). However, to date, effects of trivalent ions, Fe^{3+} and Al^{3+}, on the thermodynamic properties of PPv are still unclear. In this work, by using the same methods with previous works, the structural, electronic, magnetic, and thermodynamic properties of $(Mg,Fe^{3+})(Si,Fe^{3+})O_3$ and $(Mg,Fe^{3+})(Si,Al^{3+})O_3$ PPv at several pressures, from 0 GPa to 180 GPa, are investigated. Our results show that for $(Mg,Fe^{3+})(Si,Fe^{3+})O_3$ PPv, Fe^{3+} ions substituted at Mg and Si site respectively have the high and low spin state within the deep LM pressure range, while Fe^{3+} in $(Mg,Fe^{3+})(Si,Al^{3+})O_3$ PPv remains in the high spin state. Furthermore, separated phase between Fe_2O_3 and Al_2O_3 in PPv is found unfavorable.

References:
[1] Metsue, A. and Tsuchiya, T. (2012) Geophys. J. Int. **190**, 310.
[2] Tsuchiya, T. and Wang, X. (2013) J. Geophys. **118**, 83.
[3] Wang, X. and Tsuchiya, T. To be submitted.
[4] Metsue, A. and Tsuchiya, T. (2011) J. Geophys. Res. **116**, B08207.

キーワード: First-principles method, Internally consistent LSDA+U, Thermodynamic properties, Postperovskite
Keywords: First-principles method, Internally consistent LSDA+U, Thermodynamic properties, Postperovskite