Toward the unified image of the spin transition of iron in the lower mantle minerals

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Pressure-induced spin transition of iron in the lower mantle minerals is important to understand the dynamics of the lower mantle. However, we still do not have the unified image of the spin transition of iron in Mg-perovskite (Pv) and post-Mg-perovskite (PPv). The prolonged controversy of the spin state of Fe^{2+} in Pv and PPv seems to have settled down that Fe^{2+} remains high spin (HS) at the dodecahedral site (A site). However, there is still a controversy about the preferred site and the spin state of Fe^{3+} in Al-bearing Pv and PPv. Some experimental results indicate that Fe^{3+} becomes low spin (LS) at the octahedral site (B site) in Al-bearing Pv and PPv that involve no Fe^{2+} [1] [2]. On the other hand, other experimental results indicate that Fe^{3+} prefers to occupy the A site and remains HS in Pv and PPv that involve a certain amount of Fe^{2+} [3] [4]. First-principles calculations also indicate that Fe^{3+} remains HS at the A site [5].

In an attempt to resolve these situations, we are trying to find the reasons to explain these discrepancies. So far, in the previous reports, Fe^{3+} is assumed to occupy the regular A or B site with space group *Pbnm* (Pv) or *Cmcm* (PPv). However, there is a possibility that Fe^{3+} may occupy the locally distorted site although the space group remains *Pbnm* (Pv) or *Cmcm* (PPv), and these possibilities have not yet been fully examined experimentally or theoretically. Also, coexisting Fe^{2+} at the A site may affects the preferred site and thereby the spin state of Fe^{3+} in Pv and PPv. In the presentation, these possibilities are discussed to resolve the above discrepancies and obtain the unified image of the spin transition of iron in the lower mantle minerals.

[1] Catalli et al. (2011) *EPSL* **310**, 293-302. [2] Fujino et al. (2014) *PEPI* **228**, 186-191. [3] Mao et al. (2014) *EPSL* **403**, 157-165. [4] Dorfman et al. (2014) *2014 AGU Fall Meeting*, MR24A-01. [5] Hsu et al. (2012) *EPSL* **359-360**, 34-39.