

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

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The pressure-induced spin transition of iron in the lower mantle minerals deeply affects the structures and physical properties of the lower mantle minerals, and thereby the dynamics of the lower mantle. So far, many experimental and theoretical studies have been carried out to clarify the spin transition of iron in the lower mantle minerals. However, there is still a controversy about the existence and the pressure dependence of the spin transition of iron in Mg-perovskite (Pv) and post-Mg-perovskite (PPv) at the lower mantle conditions. Pv and PPv in the lower mantle are considered to involve both Fe²⁺ and Fe³⁺, and Al as minor elements. Until recently, the controversy had been mainly about the spin transition of Fe²⁺. Now, the spin transition of Fe²⁺ in Pv and PPv seems to be settling down in the direction that Fe²⁺ in both Pv and PPv remains high spin (HS) at the dodecahedral site (A site) at the lower mantle conditions (Hsu et al., 2011; Yu et al., 2012).

On the other hand, with the spin transition of Fe³⁺ there are still large discrepancies among the reports, particularly related to the Al content involved in Pv and PPv. Some experimental results indicate that Fe³⁺ becomes low spin (LS) at the octahedral site (B site) in Al-bearing Pv (above ca. 70 GPa) and PPv (whole stability region) (Catalli et al., 2011; Fujino et al., 2012, 2013), while other experimental results indicate that Fe³⁺ coexisting with Fe²⁺ at the A site prefers to occupy the A site and remains HS even at high pressure (Mao et al., 2014; Dorfman et al., 2014). Meanwhile first-principles calculations indicate that Fe³⁺ remains HS at the A site in Al-bearing Pv and PPv (Hsu et al., 2012).

In the presentation, the possible explanations to resolve the above discrepancies among the previous reports to obtain the unified image of the spin transition of iron in the lower mantle minerals are proposed.

Keywords: spin transition of iron, ferric iron, Mg-perovskite, post-Mg-perovskite, Al content, cation exchange reaction