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Spin transitions of iron in the lower mantle minerals - new approaches to settle the spin transition problems of iron -

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Although pressure-induced spin transition of iron is very important to understand the mineralogy and dynamics of the lower mantle, spin transitions of iron in the lower mantle minerals have long been unclear except for ferropericlase. In particular, the spin transition of iron in Mg-perovskite (Pv) has been the issue of a lot of controversy. However, very recently there is a sign that this chaotic state of spin transition problems of iron in Pv will be improved or settled through the following two approaches. One is through the theoretical works on quadrupole splitting (QS) of Fe^{2+} at the A-site in Mossbauer spectra and the other is through the experimental works on cation exchange reaction of Fe^{3+} and Al between the A- and B-sites. We are contributing to the latter approach. This time I will talk about these two approaches to the spin transition problems of iron in the lower mantle minerals.

We measured spin states of Fe^{3+} in Al-bearing Pv and post-Mg-perovskite (PPv) by X-ray emission spectroscopy (XES) and X-ray diffraction (XRD) using the well qualified samples. XES and XRD of Pv indicate that high spin (HS) Fe^{3+} occupies the A-site below 50-60 GPa but above 50-60 GPa Fe^{3+} replaces Al at the B-site by cation exchange reaction and becomes low spin (LS), while Fe^{3+} remaining at the A-site is HS up to 200 GPa. Meanwhile XES and XRD of PPv indicate that LS Fe^{3+} occupies the B-site above around 110 GPa, suggesting that cation exchange reaction of Fe^{3+} and Al between the A- and B-sites occurs below around 110 GPa. The important point here is that the spin state of Fe^{3+} is not determined only by pressure and temperature but also determined by the synthesis and annealing conditions of the samples, and cation exchange reaction of Fe^{3+} and Al between the A- and B-sites plays an important role on it.

As the other approach, Bengtson et al. (2009) and Hsu et al. (2010) reported, based on *ab initio* simulations, that high QS of Fe^{2+} at the A-site in Mossbauer spectra of Pv, which has long been used as the evidence of the intermediate spin (IS) or LS state of Fe^{2+} in the previous reports, is attributed to the HS state of Fe^{2+} at the A-site, just opposite assignment to that of the previous reports. In the presentation, based on these new approaches, spin transitions of iron in the lower mantle minerals are discussed.

Keywords: spin transition, ferric iron, Mg-perovskite, post-Mg-perovskite, X-ray emission spectroscopy, cation exchange reaction