Spin transition of ferric iron in Mg-perovskite

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Pressure-induced high-low spin transition of iron in the Earth's lower mantle has large effects on the structure and physical properties of iron-bearing Mg-perovskite (Mg-pv) and on the partitioning of iron between iron-bearing phases in the lower mantle. We measured the spin state of ferric iron in Mg-pv at the lower mantle conditions by X-ray emission spectroscopy (XES) at BL-12XU of SPring-8. Ferric iron was measured because the recent studies indicate that ferric is more dominant than ferrous for iron in Mg-pv. The composition of Mg-pv samples used for the XES measurement is $Mg_{0.85}Fe^{3+}{}_{0.15}Al_{0.15}Si_{0.85}O_3$, where Fe^{3+} and Al are thought to occupy the dodecahedral (A) site and octahedral (B) site, respectively. The emitted Fe *k beta* spectra of ferric iron in Mg-pv were measured at pressures up to 113 GPa and room temperature using the diamond anvil cells.

The obtained XES pattern of ferric iron in Mg-pv at 50 GPa was similar to that at 0 GPa. However, at 80 GPa the *k beta'* peak became lower than those at 0 and 50 GPa, and the similar XES patterns continued with increasing pressure up to 113 GPa, where the *k beta'* peak showed that ferric iron is still not at the low spin state, as compared with the XES pattern of low spin Fe^{3+} in Fe_2O_3. The preliminary calculation of the spin numbers of ferric iron in Mg-pv at 80-113 GPa gives the intermediate values between 5/2 (high spin) and 1/2 (low spin). These intermediate spin states of ferric iron in Mg-pv at the above pressure region can be explained by the crystal field splitting of the energies of 3d electrons of ferric iron at the distorted dodecahedral (A) site of Mg-pv.