Chemical reactions between Fe and H_2O up to megabar pressures and implications for water storage in the Earth’s mantle and core

*Liang Yuan[1], Eiji Ohtani[1,2], Daijo Ikuta[1], Seiji Kamada[1], Jun Tsuchiya[3], Naohisa Hirao[4], Yasuo Ohishi[4], Akio Suzuki[1]

1. Tohoku Univ., 2. Sobolev Institute of Geology and Mineralogy, Siberian Branch of RAS, 3. Ehime Univ., 4. JASRI

We investigated the phase relations of the Fe-H_2O system at high pressures based on in situ X-ray diffraction experiments and first-principles calculations and demonstrate that FeH*x* and FeO are present at pressures less than ~78 GPa. A recently reported pyrite-structured FeO_2 was identified in the Fe-H_2O system at pressures greater than ~78 GPa after laser-heating. The phase observed in this study has a unit-cell volume 8%-11% larger than that of FeO_2, produced in the Fe-O binary system reported previously, suggesting that hydrogen might be retained in a FeO_2H_x crystal structure. Our observations indicate that H_2O is likely introduced into the deep Earth through reaction between iron and water during the accretion and separation of the metallic core. Additionally, reaction between Fe and H_2O would occur at the core-mantle boundary, given water released from hydrous subducting slabs that intersect with the metallic core. Accumulation of volatile-bearing iron compounds may provide new insights into the enigmatic seismic structures observed at the base of the lower mantle.

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