Chemical reactions between Fe and H\textsubscript{2}O up to megabar pressures and implications for water storage in the Earth’s mantle and core

*Liang Yuan\textsuperscript{1}, Eiji Ohtani\textsuperscript{1,2}, Daijo Ikuta\textsuperscript{1}, Seiji Kamada\textsuperscript{1}, Jun Tsuchiya\textsuperscript{3}, Naohisa Hirao\textsuperscript{4}, Yasuo Ohishi\textsuperscript{4}, Akio Suzuki\textsuperscript{1}\textsuperscript{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\textsubscript{2}O system at high pressures based on in situ X-ray diffraction experiments and first-principles calculations and demonstrate that FeH\textsubscript{x} and FeO are present at pressures less than ~78 GPa. A recently reported pyrite-structured FeO\textsubscript{2} was identified in the Fe-H\textsubscript{2}O 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\textsubscript{2}, produced in the Fe-O binary system reported previously, suggesting that hydrogen might be retained in a FeO\textsubscript{2}H\textsubscript{x} crystal structure. Our observations indicate that H\textsubscript{2}O 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\textsubscript{2}O 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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