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Experimental investigation of phase relations in the Fe-O-H system under high pressure-temperature conditions: implications for hydrogen-oxygen deep cycles

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Experimental investigation of phase relations in the Fe-O-H system under high pressure-temperature conditions: implications for hydrogen-oxygen deep cycles

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We investigated phase relations in the Fe-O-H system based on in-situ synchrotron x-ray diffraction measurements and observed formation of a series of mixed-valence iron oxides under high pressure-temperature (*P*-*T*) conditions of the lower mantle. Wustite ($Fe_{1-x}O$) or hematite (Fe_2O_3) was used as the starting materials, and synthetic SiO_2 gel (containing ~2 wt.% H_2O) or deionized water was loaded as pressure medium and water supply. In runs using hydrous SiO_2 gel to control the water content, hematite transformed into the high-pressure phase of magnetite (Hp-Fe_3O_4)[1] and a new hydrous hexagonal phase ($Fe_{12.76}O_{18}H_x$, denoted as "HH1-phase") at 45 GPa and 66 Gpa, respectively. Meanwhile, wustite transformed into a mixed-valence iron oxide $Fe_{25}O_{32}$ with a hexagonal lattice[2][3] above 78 GPa and 2000 K. In other runs loaded with saturated water, the HH1-phase or pyrite-structured $FeOOH_x$ ($_x$<1, Py-phase) was the stable phase independent on the iron valence state of the starting materials.

Formation of mixed-valence iron oxides and hydroxides suggests that the phase diagram in Fe-O-H system under high *P*-*T* conditions is more complex than previously thought. Future research should focus on understanding the role of water in the processes of deep oxygen-hydrogen cycle in the deep mantle.

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