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Hydrogen occupation and hydrogen-induced volume expansion in $Fe_{0.9}Ni_{0.1}D_x$ at high *P-T* conditions

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Abstract

The density of the Earth's core is several percent lower than that of iron-nickel alloy under conditions of pressure and temperature equivalent to the Earth's core. Hydrogen is one of the most promising constituents accounting for the density deficit, but hydrogen occupation sites and density decrease of iron-nickel alloy caused by hydrogenation have never been investigated. In this study, the phase relation and crystal structure of $Fe_{0.9}Ni_{0.1}H_x(D_x)$ at high pressures and temperatures up to 12 GPa and 1000 K were clarified by in situ X-ray diffraction and neutron diffraction measurements. Under the *P-T* conditions of the present study, no deuterium atoms occupied tetragonal (*T*) sites of face-centered cubic (fcc) $Fe_{0.9}Ni_{0.1}D_x$, although the T-site occupation was previously reported for fcc $FeH_x(D_x)$. The deuterium-induced volume expansion per deuterium v_D was determined to be 2.45(4) and 3.31(6) Å^3 for fcc and hcp $Fe_{0.9}Ni_{0.1}D_x$, respectively. These v_D values are significantly larger than the corresponding values for FeD_x. The v_D value for fcc $Fe_{0.9}Ni_{0.1}D_x$ slightly increases with increasing temperature. This study suggests that only 10% of nickel in iron drastically changes the behaviors of hydrogen in metal. Assuming that v_D is constant regardless of pressure, the maximum hydrogen content in the Earth's inner core is estimated to be one to two times the amount of hydrogen in the oceans.

Keywords: Neutron diffraction, high pressure, metal hydride, Earth's core; Physics and Chemistry of Earth's Deep Mantle and Core