# Pressure-volume-temperature relations for hydrogen volume and content in iron hydride at high pressure and high temperature

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The Earth's core has supposed to be constituted by iron, nickel and some light elements. In order to elucidate the property of the Earth's core, many studies to quantify the content of light elements in the Earth's core has been progressed through sound velocity and magnetic measurements, or theoretical research. Hydrogen is one of the most probable candidate among the light elements constituting the Earth's core due to the relations between iron and hydrous melt in the magma ocean in the early Earth, and the discovery of the post-perovskite phase and that melting temperature. Although several studies on iron hydride ($FeH_x$) have been conducted, precise measurement of hydrogen content in metallic iron under high pressure and high temperature conditions has not been conducted due to the difficulty of the experiment. Hydrogen cannot be directly observed by traditional methods such as x-ray diffraction method. On the other hand, in neutron diffraction experiments, most of the direct observations of hydride has been carried out through substitution from hydrogen to deuterium because hydrogen has strong incoherent scattering. Therefore in many previous studies, the volume and the content of the hydrogen in metallic iron are assumed through the studies of several metallic hydride. However, such assumptions without precise measurement cause uncertainty, for example, when deriving the hydrogen content from the volume of $FeH_x$. In this study, to determine the hydrogen content and volume at high pressure and high temperature, high pressure neutron diffraction experiment for $FeH_x$ was conducted under nearly isobar condition at 5-6 GPa and 8-9 GPa up to 1100 K in BL11 beamline, J-PARC. The phase transition and hydrogenation of iron were observed by dhcp-$FeH_x$ and fcc-$FeH_x$ phases, which are high pressure and high temperature phase of $FeH_x$. The structure of $FeH_x$ and the content of hydrogen were determined by Rietveld refinement. The content of hydrogen $x$ was obtained to 1.0-0.5, which is decreased by increasing temperature. We report the relations between the volume and the content in $FeH_x$ at high pressure and high temperature.

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