Fcc FeH_x at core pressure

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Hydrogen is one of the plausible candidates of light element(s) in the Earth's core. Previous studies suggested that hydrogen preferentially partitioned into liquid metallic iron core as FeH_x in the magma ocean of the primordial Earth. [e.g., 1,2]. *In-situ X-ray* diffraction experiments revealed that FeH_x with double-hexagonal close packed (dhcp) structure formed at 3.5 GPa and the structure did not change up to at least 80 GPa [3,4]. Energetic calculations indicate the structural transition of dhcp to hexagonal close packed (hcp), and hcp to face-centered cubic (fcc) structure at the Earth's lower mantle pressure [5]. However, the suggested phase transitions of FeH_x has not been verified by experiments, and therefore the crystal structure of FeH_x under core pressures is still an open question.

We examined the phase relations of FeH_x at high pressures and high temperatures in a laser-heated diamond-anvil cell based on synchrotron X-ray diffraction measurements at BL10XU, SPring-8. The results show that dhcp-FeH_x disappeared and hcp-FeH_x formed at ~60 GPa, and hcp-FeH_x underwent transformation into fcc-FeH_x at ~70 GPa. We also obtained the pressure-volume (*P-V*) data of fcc-FeH_x at 26 to 137 GPa and 300 K. The compressivity showed a discontinuous change at ~70 GPa, which may be induced by a magnetic transition of fcc-FeH_x, as indicated by the theoretical calculation [5]. Based on our experimental results, we argue that a likely crystal structure of FeH_x at the Earth's core conditions is fcc structure rather than dhcp and hcp.

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