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Fcc FeHx at core pressure

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Hydrogen is one of the most important candidates of light element(s) of the components the core of the Earth which explain the density deficit of the core. During the core formation, hydrogen preferentially dissolved into the metallic core as FeHx (e.g. Fukai, 1984; Okuchi et al., 1997). However, the phase diagram of FeHx is limited to relatively low pressure (Sakamaki et al., 2009), and its crystal structure under core pressure and temperature has not been revealed. Energetic calculations indicate the transition of double-hexagonal close packed (dhcp) to hexagonal close packed (hcp), and hcp to face-centered cubic (fcc) structure at lower mantle pressure (Isaev et al., 2007), but it has not been verified by experiments. We examined the phase transition from dhcp- or hcp-FeHx to fcc-FeHx by high-pressure and temperature experiments using laser-heated diamond-anvil cell technique and synchrotron X-ray diffraction measurements at SPring-8. It was revealed that dhcp-FeHx disappeared and hcp-FeHx formed at ˜60 GPa, and hcp-FeHx transformed into fcc-FeHx at ˜70 GPa. The compression behavior of fcc-FeHx was also obtained at 26 to 137 GPa. The pressure-volume relations and the compressivity showed an almost discontinuous change at ˜70 GPa, which may reflect the magnetic transition of fcc-FeHx, as indicated by theoretical calculations in Isaev et al., 2007. According to these results, the structure of FeHx at core conditions of the Earth may be fcc rather than dhcp.

Keywords: core, hydrogen, fcc structure, high pressure, X-ray diffraction