The effects of ferromagnetism and interstitial hydrogen on the equation of states of hcp FeH_x

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Hydrogen is one of the important candidates of the light elements of the Earth’s core, because only a small amount of interstitial hydrogens may drastically change the physical properties of compressed iron (e.g. melting temperature, density and elastic properties). Since the solubility of hydrogen has strong pressure dependence, hydrogen content must be determined by in-situ observations. Combined with X-ray diffraction measurements, the following relation is widely used for this purpose: $x = (V_{FeHx} - V_{Fe}) / V_H$, where x is the hydrogen content, V_H is the volume expansion caused by unit concentration of hydrogen, V_{FeHx} and V_{Fe} are volumes of FeH_x and pure iron, respectively (Fukai, 1992). Ambient pressure experiments on many face-centered cubic (fcc) metals suggest that V_H is insensitive to the hydrogen content x. However, it has not been confirmed for compressed iron. We computed the equation of states of hexagonal-closed pack (hcp) iron with interstitial hydrogen with x = 0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9 and 1.0 by using the AkaiKKR firstprinciples package. Coherent potential approximation (CPA) was adopted to treat non-saturated hydrogen atoms, which randomly occupied the octahedral sites. The results of pure (x = 0.0) and hydrogen saturated (x = 1.0) iron are consistent with previous experiments (Hirao et al., 2004; Narygina et al., 2011). However, we found a discontinuous volume change as functions of hydrogen content for non-saturated FeH_x because of the ferromagnetic transition. We also found almost no x dependence on the volume in the ferromagnetic phase. Previous Mossbauer spectroscopy measurements suggest the ferromagnetic state is stable up to about 25 GPa for iron hydride (Mitsui et al., 2010; Narygina et al., 2011). This means that previous experiments possibly overestimate the hydrogen content of ferromagnetic FeH_x.

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