Formation of non-stoichiometric fcc and hcp FeHx at high pressure and temperature conditions

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Abstract

Hydrogen is one of the likely light elements in the Earth's core but the phase relation of FeHx alloy is not well known yet, due to experimental difficulties. Double hexagonal closed packed (dhcp) FeH was suggested to be stable, at least to 136 GPa based on static compression at room temperature, whereas the stabilities of face centered cubic (fcc) and hcp FeHx were also reported. The phase relation in FeHx, in particular for a hydrogen depleted composition (x< 1) and at high temperatures, remains to be examined. Here we performed experiments on FeHx (x< 1) using a laser-heated diamond anvil cell (LH-DAC) and observed its phase relation up to 136 GPa and 2000 K by X-ray diffraction measurements. Rhenium gasket was used without hydrogen sealing; that is, system was open for hydrogen. Dhcp FeHx (x_˜1) was synthesized under 5 GPa by annealing. However, the diffraction peaks from dhcp FeH became weak over 20 GPa, and then dhcp to fcc phase transition took place up to 33 GPa, in which x = 0.9 to 1.0. With further compression, the fcc phase was preserved, although x decreased to 0.7 at 93 GPa. During heating below 1800 K at 65, 70, and 122 GPa, hcp FeHx formed and the fcc phase gradually disappeared probably because of hydrogen escape from a sample chamber. The amount hydrogen in this hcp phase was lower than 0.6 and decreased with increasing laser output power. Our result indicated that both fcc and hcp phases could have stability fields in the Fe-H binary system. Because hydrogen concentration required to account for the density deficit is 0.6 (_˜1 wt.% H) in the outer core and 0.1 in the inner core, hcp FeHx is the most important compound in order to test the hypothesis that hydrogen is in the Earth's core.

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