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Stability of fcc phase FeH to 137 GPa

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Abstract

We examined the crystal structure of FeH_X (X~1) (FeH hereafter) at high pressure and temperature by X-ray diffraction up to 137 GPa. Results show that FeH adopts a face-centered cubic (fcc) structure at pressures of 43 to 137 GPa and temperatures of ~1000 to 2000 K. Our study revises a phase diagram of stoichiometric FeH in which fcc has a wider-than-expected stability field at high pressure and temperature. Based on our findings, the FeH end-member of the Fe-FeH system is expected to be stable in the fcc structure at the *P-T* conditions of the Earth's core, rather than in the double-hexagonal close packed (dhcp) structure as previously reported. We compared the experimentally determined unit-cell volumes of FeH with those from ab initio calculations. Additionally, we observed a change in compressibility at ~60 GPa, which could be attributed to a magnetic transition—an interpretation supported by our ab initio computations.

Keywords: FeH, fcc structure, Earth's core, X-ray diffraction, ab initio calculation