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Hydrogen solubility in FeSi alloy phases at high pressures and temperatures

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Abstract

Light elements alloying with metallic Fe can change the properties and therefore play a key role in the structure and dynamics of planetary cores. Hydrogen and silicon are possible light elements in the rocky planets' cores. However, hydrogen storage in Fe-Si alloy systems remains unclear at high pressures and high temperatures because of experimental difficulties. Taking advantage of pulsed laser heating combined with high-energy synchrotron X-ray diffraction, we studied reactions between FeSi and H in laser-heated diamond-anvil cells (LHDACs) up to 61.9 GPa and 3500 K. We found that under H-saturated conditions the amount of H alloying with FeSi (0.3 and <0.1 wt% for the B20 and B2 structures, respectively) is much smaller than that in pure Fe metal (>1.8 wt%). Our experiments also suggest that H remains in the crystal structure of FeSi alloy when recovered to 1 bar. Further density functional theory (DFT) calculations indicate that the low-H solubility likely results from the highly distorted interstitial sites in the B20 and B2 structures, which are not favorable for H incorporation. The recovery of H in the B20 FeSi crystal structure at ambient conditions could open up possibilities to understand geochemical behaviors of H during core formation in future experiments. The low-H content in FeSi alloys suggests that if a planetary core is Si-rich, Si can limit the ingassing of H into the Fe-rich core.

Keywords: FeSi alloy, hydrogen content, planetary cores, pulsed-laser heating, synchrotron X-ray diffraction