Hydrogen solubility in FeSi alloy phases at high pressures and temperatures

SUYU FU1,*, STELLA CHARITON2, VITALI B. PRAKAPENKA2, ANDREW CHIZMESHYA3, AND SANG-HEON SHIM1,*

1School of Earth and Space Exploration, Arizona State University, Tempe, Arizona 85287, U.S.A.
2Center for Advanced Radiation Sources, University of Chicago, Chicago, Illinois 60637, U.S.A.
3School of Molecular Sciences, Arizona State University, Tempe, Arizona 85281, U.S.A.

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

INTRODUCTION

In recent decades, finding habitable planets has drawn interest from not only astrobiologists and astrophysicists but also Earth scientists. Studies indicate that in addition to atmosphere and surface conditions, the interior of a planet could play a key role in its habitability (Shahar et al. 2019). For instance, the dynamo generated by the core could affect the habitability of the surface environment. Light elements are believed to partition into the Fe metal core during the early magma ocean stage of planets (Stevenson 2003) and can greatly affect the properties, such as phase relation and melting behavior (Hirose et al. 2013). Considering the diverse sizes and masses of planets found in the solar system and the exo-planetary systems (Batalha et al. 2011; Jontof-Hutter et al. 2015), from Mars-size rocky planets to gas giants, it is key to studying Fe with light elements for a wide range of pressures.

Hydrogen is the most abundant element in the universe (Anders and Grevesse 1989; Grevesse and Sauval 1998). A large amount of H, more than 1.8 wt%, can dissolve into solid Fe metal at high pressures (Badding et al. 1991; Pépin et al. 2017). Sakamaki et al. (2009) showed that alloying with H can lower the melting temperature of Fe by as much as 600–900 K below 20 GPa. In some models, Si is thought to be the most abundant light element in the Earth’s core, up to 12 wt% (Li and Fei 2003; Hirose et al. 2013). Based on the S/Si ratio and the FeO content of Mercury’s surface, its core could contain more than 12 wt% Si (Nittler et al. 2011; Knibbe and van Westrenen 2018). Therefore, it is important to include Si in Fe metal to understand the impact of H on the constituent phases of the planetary cores.

Studies on the H content in the Fe-Si system are limited to low pressures and/or low temperatures. For instance, Tagawa et al. (2016) conducted laser heating on Fe0.88Si0.12 (6.5 wt% Si) in a H medium at 27 and 62 GPa using DACs, and found that about 1.2–1.5 wt% H can be incorporated into the hexagonal-close-packed (hcp) alloy. However, the heating was conducted below ~1000 K. In addition, a multi-anvil experiment reported a much lower H solubility of 0.2–0.3 wt% in the B20-structured FeSi alloys up to 20 GPa and 2000 K (Terasaki et al. 2011), where the pressure was, however, not sufficiently high for rocky planets’ cores greater than that of Mars.

Despite its importance, studying H in LHDACs has been difficult because of its fast diffusion into diamond anvils, which can make them brittle. The embrittlement problem becomes more severe with heating. Recently, pulsed laser heating combined with gated synchrotron X-ray diffraction (XRD) enabled the heating of H to thousands of kelvins in LHDACs ( Goncharov et al. 2010). By taking advantage of the development, we have studied reactions between H and FeSi alloy phases in a H-saturated condition up to 61.9 GPa and 3500 K. We have