Hydrogen Storage in FeSi Alloy at High Pressure: Implications for the Composition and Structure of Rocky Planets' Cores. S. F. Suyu Fu [1] and S. H. S. Sang-Heon Shim[2], [1] School of Earth and Space Exploration, Arizona State University, Tempe, AZ 85287, United States (suyufu@asu.edu) for first author, [2] School of Earth and Space Exploration, Arizona State University, Tempe, AZ 85287, United States (sshim5@asu.edu).

Introduction: The composition and structure of planets' interiors play a key role on its dynamic evolution and further surface habitability [1, 2]. Light elements may be the key ingredients for the generation of global-scale dynamo for rocky planets [3-5]. The light elements can also alter properties of metallic iron, including melting points, phase relations, and density. Recent studies have shown that pure Fe and Fe-Ni alloys can store a large amount of H in their crystal structures with a H/Fe molar ratio as high as 1-5 depending on pressure and temperature (P-T) conditions [6-8]. However, the hydrogen storage in iron alloys with other light element candidates, such as Si and S, have not been well studied [9]. Here we report high-pressure experiments on reactions between stoichiometric FeSi alloy and hydrogen up to 45 GPa and 3000 K in laser-heated diamond anvil cells. We monitored the chemical reaction and crystal structures of products using in situ X-ray diffraction at high P-T. We found that B20-structured FeSi alloy exhibits systematically larger unit-cell volume by 4-5% when it is heated in a hydrogen medium at high pressure. Based on our first-principles calculations, we estimate that the B20 FeSi can store up to 20-30 mol% H in its crystal structure, which is much less than those observed in pure Fe or Fe-Ni alloys [6-8]. In our experiments, the higher-pressure BCC polymorph of FeSi showed no unit-cell volume expansion up to 45 GPa, suggesting little or no hydrogen storage in the BCC phase. Our observations thus indicate that the existence of Si in Fe will significantly reduce the hydrogen storage capacity of Fe alloys. Therefore, the abundance of Si in rocky planets' cores could control the hydrogen incorporation over the early evolution process. In addition, the interplay between H and Si in Fe alloys we found at high P-T can impact partitioning behaviors of H and Si between the silicate mantle and the metallic core of rocky planets, increasing the Mg/Si ratio of the silicate mantle and the amount of H partitioning into the mantle over the core in some rocky planets.

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