2 Laboratory Studies of Crystalline FeSi to 47 GPa and 2800 K

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Introduction

Equations of state, melting curves, mixing relations and solid-solid phase boundaries in iron and its alloys are the key equilibrium properties needed for modeling the constitution and evolution of planetary cores. Silicon is one element that is likely to be alloyed with iron in the cores of rocky planets; it is abundant in the rocks found on the surfaces of Mercury, Venus, Earth and Mars (de Pater and Lissauer, 2010), and in the laboratory it is known to alloy with liquid iron at high pressures (Sanloup and Fei, 2004) or at low oxygen fugacity (McCoy et al., 1999).1

Recently, the cubic ε-phase of FeSi was found to transform to another cubic phase, B2, at 24 GPa and high temperature (Dobson et al., 2002)—conditions that exist in the cores of Mars and Mercury. Yet several properties of the ε to B2 phase transition remain uncertain, including the location of the phase boundary in pressure-temperature space, and the entropy difference between the two phases.

Here we present X-ray diffraction data of hot, dense FeSi. First, we show that it remains solid up to at least 2350 ± 200 K at 23 GPa and 2770 ± 200 K at 47 GPa, which means that addition of silicon does not cause a large amount of melting point depression (the melting temperature of pure iron ranges from 2300 ± 100 K to 2700 ± 150 K between 20 and 50 GPa). Second, the ε to B2 crystal-crystal phase transition occurs at 30 ± 2 GPa at all temperatures from 1200 K to 2300 K. It results in a 5% density increase, which may cause an increase in the miscibility of silicon in iron at P > 30 GPa, with potential implications for the cores of small rocky planets such as Mars and Mercury.

Experimental Method

Stoichiometric FeSi was synthesized and given to us by Ravhi S. Kumar. It was ground to a fine powder and loaded into diamond anvil cells with rhenum gaskets. The samples were surrounded with an argon or neon pressure transmitting medium. High-pressure samples were laser-heated at GeoSoilEnviroCARS (GSECARS) end-station ID-D, and simultaneous emission spectra and X-ray diffraction images were collected (Prakapenka et al., 2008).

Details of temperature and pressure measurements and of their uncertainties will be presented in an upcoming publication.

Results and Discussion

The solid-solid phase transition from the low pressure ε phase to the high pressure B2 phase of FeSi occurs at 30 ± 2 GPa, the weighted average of the transition pressures detected in a neon pressure medium (31.2 ±1.7 GPa) and in an argon medium (28 ±1.9 GPa) (Figure 2.2.1). We detected no temperature dependence of the ε-B2 transition in either pressure medium, despite controlling the temperature at 1200 ± 100 K for tens of seconds before increasing laser power: either the sample started transforming immediately upon heating to 1200 K, or it did not transform until pressure was increased. The ε-B2 transition was reversed multiple times in each pressure medium. Examples of the X-ray diffraction spectra that evidence the transition are shown in Figure 2.2.2. To constrain the hysteresis of the phase transition, we reversed the transition four times in a cell containing the neon pressure medium, and twice in a cell containing the argon medium. The reversals in neon showed no evidence of hysteresis once they were laser-heated, but rather bracket the

1. Much of this report is quoted from a manuscript submitted to American Mineralogist: paper #4612R
The transition to between 30 and 32 GPa. The reversals in argon, on the other hand, show hysteresis—upon laser-heating, the B2 phase is created at 32 GPa, transformed into the phase at 23 GPa on decompression, and transformed back into the B2 phase at 30 GPa upon re-compression.

X-ray diffraction patterns of samples at room temperature provide data to constrain the P-V equation of state of both phases of FeSi and show that density increases by 5% during the phase transition at 30 GPa, which may have implications for the cores of Mercury (P_{core} ~ 10 to 40 GPa) and/or Mars (P_{core} ~ 24 to 40 GPa) if silicon is an abundant alloying element. Qualitatively, the miscibility of silicon in crystalline iron may increase at ~30 GPa due to the increase in the effective hard sphere radius of silicon in the FeSi lattice as its coordination changes from 7-fold (ε-phase) to 8-fold (in the B2 structure), thereby improving the similarity of the radii of silicon and iron. Specifically, the immiscibility gap documented between iron-rich and iron-poor iron-silicon alloys at < 50 mol% Si may be reduced at pressures above 30 GPa.

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References