Composition-dependent thermal equation of state of B2 Fe-Si alloys at high pressure

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**ABSTRACT**

Solid iron-silicon alloys play an important role in planetary cores, especially for planets that formed under reducing conditions, such as Mercury. The CsCl (B2) structure occupies a considerable portion of the Fe-Si binary phase diagram at pressure and temperature conditions relevant for the core of Mercury, yet its thermodynamic and thermoelastic properties are poorly known. Here, we report in situ X-ray diffraction measurements on iron-silicon alloys with 7–30 wt% Si performed in laser-heated diamond-anvil cells up to ~120 GPa and ~3000 K. Unit-cell volumes of the B2 phase at high pressures and high temperatures have been used to obtain a composition-dependent thermal equation of state of this phase. In turn, the thermal equation of state is exploited to determine the composition of the B2 phase in hcp+B2 mixtures at 30–100 GPa and to place constraints on the hcp+B2/B2 phase boundary, determined to vary between ~13–18 wt% Si in the considered pressure and temperature range. The hcp+B2/B2 boundary of Fe-Si alloys is observed to be dependent on pressure but weakly dependent on temperature. Our results, coupled with literature data on liquid equations of state, yield an estimation of the density contrast between B2 solid and liquid under Mercury’s core conditions, which directly relates to the buoyancy of the crystallizing material. While the density contrast may be large enough to form a solid inner core by the gravitational sinking of B2 alloys in a Si-rich core, the density of the B2 solid is close to that of the liquid at solidus conditions for Si concentration approaching ~10 wt% Si.

**Keywords:** Fe-FeSi system, equation of state, phase diagram, high-pressure experiment, planetary interiors, Mercury, inner core

**INTRODUCTION**

The abundance of metallic iron and silicate minerals in telluric planets leads to the expectation that iron-silicon alloys play a large role in planetary cores when formed under reducing conditions (Kilburn and Wood 1997; Ricollet et al. 2011). Varying quantities of silicon alloyed with iron have been invoked to explain seismological observations of Earth’s core (e.g., Fischer et al. 2012; Badro et al. 2015; Antonangeli et al. 2018) and geodetic observations of Mercury (e.g., Knibbe and van Westrenen 2018; Genova et al. 2019; Terasaki et al. 2019). To accurately model the interior structure and dynamics of these planets, the phase diagram of Fe-Si alloys at high pressure (P) and high temperature (T) and the thermal equations of state (EoS) of stable phases are crucial. In particular, the high Si/Si ratio and low FeO content of Mercury’s surface indicate that its interior is likely to be highly reduced (Nittler et al. 2011), leading to expected bulk core Si concentrations in excess of 12 wt% Si (Chabot et al. 2014; Knibbe and van Westrenen 2018; Terasaki et al. 2019). Consequently, the chemical and elastic properties of Si-rich Fe-Si alloys are key to understanding the present state and dynamics of Mercury’s core.

Iron-silicon alloys at ambient pressure exhibit a complex phase diagram, with a series of solid solutions over a wide compositional range, in addition to several stoichiometric compounds such as FeSi, FeSi₁₋₂, and Fe₂Si (Cui and Jung 2017). Stoichiometric FeSi has a B20 structure at ambient conditions (FeSi is the B20 structure prototype) and transforms into a B2 (CsCl type) structure at pressures above 30–40 GPa at high T (Fischer et al. 2013; Geballe and Jeanloz 2014). On the other side, at these pressures, the pure Fe end-member exhibits fcc structure at high T and hcp structure at lower T, and its stability field expands by the addition of silicon (Brosh et al. 2009; Komabayashi et al. 2009, 2019). Other stoichiometric compounds in the Si-rich side of the Fe-Si system, such as Fe₂Si and Fe₃Si, are reported to be unstable with increasing P and T (Ponomareva et al. 2009; McGuire et al. 2017), although exact phase boundaries are poorly constrained. The coexistence field of B2 and hcp phases is also poorly constrained at high P-T (Kuwayama et al.