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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