
Phase transition boundary between fcc and hcp structures in the system Fe-Si and its implications for thermodynamics of silicon-bearing Earth's core

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Abstract

The phase transition between a face-centred cubic (fcc) and hexagonal close-packed (hcp) structure in Fe-Si alloys were examined in an internally resistive heated diamond anvil cell (DAC) under high-pressure (P) and -temperature (T) conditions with in-situ synchrotron X-ray diffraction (XRD). High pressure was generated in a DAC with a pair of diamond anvils with a culet size of 300 μm or 150-450 μm beveled depending on the pressure range. The starting material was Fe-4wt%Si, sandwiched between SiO₂ glass layers which served as a pressure transmitting medium and thermal insulator. High temperature was achieved with an internal resistive system. A 5-7 μm thick sample foil was placed in the sample chamber and resistively heated by directly applying a DC voltage by an external power supply. The temperature was measured by a spectral radiometric system as in conventional laser heating experiments. In-situ XRD experiments were conducted at the beamline ID27, European Synchrotron Radiation Facility. We placed tight constraints on the P-T locations and the width of the phase loop of the fcc-hcp transition. From the precisely constrained phase loop, we have constructed a thermodynamic model for the fcc-hcp transition in the Fe-Si system. The model includes P-T dependence of the mixing properties of Fe-Si alloys. We then extend the discussion to the thermodynamics of melting in the system Fe-Si. The compositions of coexisting liquid and solid (fcc or hcp) have been reported to be close (< 1 wt%Si) at pressures higher than 50 GPa, and we evaluated the thermodynamic parameters which reproduce those melting relations. We will show our experimental data and thermodynamic modelling, and then further discuss resulting implications for Earth's core.

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