Phase transition boundary between fcc and hcp structures in Fe-Si alloy and its implications for terrestrial planetary cores

TETSUYA KOMABAYASHI¹*, GIACOMO PESCE¹, GUILLAUME MORARD², DANIELE ANTONANGELI², RYOSUKE SINMYO³†, AND MOHAMED MEZOUAR⁴

¹School of GeoSciences and Centre for Science at Extreme Conditions, University of Edinburgh, EH9 3FE, U.K.
²Sorbonne Université, Muséum National d’Histoire Naturelle, UMR CNRS 7590, IRD, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, IMPMC, 75005 Paris, France
³Bayerisches Geoinstitut, Universität Bayreuth, 95440 Bayreuth, Germany
⁴European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex, France

ABSTRACT

The phase transition between a face-centered cubic (fcc) and hexagonal close-packed (hcp) structures in Fe-4wt% Si alloy was examined in an internally resistive heated diamond-anvil cell (DAC) under high-pressure (P) and high-temperature (T) conditions to 71 GPa and 2000 K by in situ synchrotron X-ray diffraction. Complementary laser-heated DAC experiments were performed in Fe-6.5wt% Si. The fcc-hcp phase transition boundaries in the Fe-Si alloys are located at higher temperatures than that in pure Fe, indicating that the addition of Si expands the hcp stability field. The dP/dT slope of the boundary of the entrant fcc phase in Fe-4wt% Si is similar to that of pure Fe, but the two-phases region is observed over a temperature range increasing with pressure, going from 50 K at 15 GPa to 150 K at 40 GPa. The triple point, where the fcc, hcp, and liquid phases coexist in Fe-4wt% Si, is placed at 90–105 GPa and 3300–3600 K with the melting curve same as in Fe is assumed. This supports the idea that the hcp phase is stable at Earth’s inner core conditions. The stable structures of the inner cores of the other terrestrial planets are also discussed based on their P-T conditions relative to the triple point. In view of the reduced P-T conditions of the core of Mercury (well below the triple point), an Fe-Si alloy with a Si content up to 6.5 wt% would likely crystallize an inner core with an fcc structure. Both cores from Venus and Mars are currently believed to be totally molten. Upon secular cooling, Venus is expected to crystallize an inner core with an hcp structure, as the pressures are similar to those of the Earth’s core (far beyond the triple point). Martian inner core will take an hcp or fcc structure depending on the actual Si content and temperature.

Keywords: Earth’s core, high-pressure, diamond-anvil cell, internal resistive heating, Fe-Si alloy

INTRODUCTION

Terrestrial core formation process has been discussed in relation to metal-silicate equilibration during accretion stage (Li and Agee 1996; Wade and Wood 2005; Siebert et al. 2013) although some recent models considered disequilibrium processes at a later stage (Rubie et al. 2011). The metal-silicate equilibration inevitably results in an impure iron-rich metallic core (Wade and Wood 2005; Siebert et al. 2013). The impurity includes nickel and several less dense elements that are also called light elements (Poirier 1994; Allègre et al. 1995).

Birch (1952) pointed out that the density of pure iron might be greater than the seismological determination for Earth’s core. Such a density deficit has been associated with the presence of light element(s), and a recent internally consistent thermodynamic model of pure iron estimated the core density deficit to be 7% for the outer core and 4.5% for the inner core (Komabayashi 2014). Other terrestrial planetary cores also likely contain light elements considering the metal-silicate partitioning during the core formation. In addition, the presence of a magnetic field found in some terrestrial planets may indicate the presence of a light element-bearing partially molten core (e.g., Sohl and Schubert 2007). Light elements would be expelled at the bottom of the liquid outer core as it is less partitioned in the solid inner core, and this would drive convection in the outer core (Stevenson et al. 1983; Lister and Buffett 1995).

Among the potential light elements, silicon is considered a plausible candidate for the terrestrial planetary cores for various reasons. (1) Silicon is the second most abundant element in the mantle and series of high-pressure (P) and high-temperature (T) experiments demonstrated that silicon and oxygen could be dissolved from mantle silicates to core melt (Takafuji et al. 2005; Ozawa et al. 2009), and then silicon is partitioned between solid and liquid during core crystallization. (2) Silicon isotopic composition of stony meteorites is different from bulk silicate Earth (Georg et al. 2007; Fitoussi et al. 2009), implying that silicon might have been partitioned into the core during core-mantle differentiation (Shahar et al. 2011; Hin et al. 2014). (3) All the core formation models based on silicate-metal equilibration inevitably have silicon as a light element in the core (Wade and Wood 2005; Rubie et al. 2011; Siebert et al. 2013).

Phase relations and equations of state (EoS) of solid phases in the system Fe-(Fe)Si have been extensively studied by both