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Phase relation of Fe-Ni-Si alloy up to 3 Mbar

Takeshi Sakai[1*], Eiji Ohtani[2], Naohisa Hirao[3], Yasuo Ohishi[3]

[1]IIAIR, Tohoku Univ., [2]Faculty of Sci., Tohoku Univ., [3]JASRI

The seismic observation reveals the anisotropic structure of the Earth's inner core [Woodhouse et al., 1986;Morelli et al., 1986]. The anisotropy of the inner core could be explained by the preferred orientation of the hexagonal close-packed (hcp) phase of iron, but its direction of orientation and the stability of hcp structure are still under debate. Stixrude and Cohen (1995) suggested that the orientation with the c-axis parallel to the Earth's rotation axis. On the other hand, Steinle-Neumann et al. (2001) reported the strong temperature dependence of the axial ratio (c/a) of hcp iron and its elasticity based on theoretical calculation and suggested that the basal planes of the hcp structure are partially aligned with the rotation axis.

The crystal structure of pure iron at the inner core condition is likely to be hcp [Tateno et al., 2010]. But the inner core is not pure iron, but it should contain about 5 wt.% of nickel [Allegre et al., 1995; MacDonough and Sun, 1995] and some amount of light elements such as silicon [Birch, 1952]. Recently the phase transition of Fe-10at.%Ni from an hcp structure to a body-centered cubic (bcc) was observed at 225 GPa and 3400 K [Dubrovinsky et al., 2007]. Moreover, it is considered that silicon is one of the most plausible candidate of the light element in the core based on the cosmochemical arguments [Allegre et al., 1995] and the chemical reactions between mantle and core [Sakai et al., 2006; Takafuji et al., 2005]. Since Fe-FeSi system shows a solid solution at Fe-rich side, the solid inner core can contain some amount of silicon in its structure [Kuwayama and Hirose, 2004]. Several reports on the phase relation of Fe-Si alloy at high pressure revealed that silicon drastically expands the stability field of the fcc phase [Asanuma et al., 2008; Lin et al., 2002]. Therefore, the effect of nickel and silicon is important to consider the crystal structure of the inner core.

Here we report the phase stability of hcp phase and the axial ratio (c/a) of $Fe_{87.9}Ni_{4.4}Si_{7.7}$ up to 307 GPa and 2780 K. We used a symmetric-type diamond anvil cell with the beveled diamond anvils of inner culet size of 30-40 ?m for high pressure generation. The crystal structure of the sample was determined by the synchrotron X-ray diffraction experiment at SPring-8 BL10XU. We did not observe other phases such as a body-centered cubic (bcc) structure. The axial ratio (c/a) of $Fe_{87.9}Ni_{4.4}Si_{7.7}$ at 300 GPa shows almost a constant value of 1.59-1.60 against temperature. The weak temperature dependency of the axial ratio of hcp Fe-Ni-Si alloy could explain the seismic wave anisotropy of the inner core with the c-axis parallel to the Earth's rotation axis.

Keywords: phase relation, anisotropy of the inner core, Laser-heated diamond anvil cell