

## Phase Relations of Iron-Nickel Alloys at Multimegabar Pressure: A Study of the Earth's Inner Core Material

Iron is believed to be the major component of the Earth's core because it is the most abundant element that satisfies the seismologically observed densities. On the basis of cosmochemical models and the studies of iron meteorites, it is generally accepted that the Earth's core also contains substantial amounts of nickel. The high-pressure behavior of iron-nickel alloys is, therefore, essential for interpreting the seismic observations and understanding the nature of the Earth's core.

The phase relation of iron at relatively low pressure has been well established.  $\alpha$ -Fe with body-centered cubic (*bcc*) structure is stable at ambient condition. It transforms to  $\gamma$ -Fe with face-centered cubic (*fcc*) structure with increasing temperature and to  $\epsilon$ -Fe with hexagonal close-packed (*hcp*) structure above  $\sim 10$  GPa at 300 K. Static compression experiments revealed that the *hcp*-Fe phase is stable at least to 300 GPa at room temperature. In contrast, the phase relation and crystal structure of iron at high pressure and temperature (*P-T*) are still highly controversial. Although many crystal structures including *hcp*, *fcc*, *bcc*, *dhcp*, and orthorhombic have been proposed as the candidate structure of iron under the Earth's core conditions, it is a matter of extensive debate. The effect of nickel on the phase relation of iron at high pressure is also not clear.

To achieve extremely high *P-T* conditions found in the Earth's core is a major experimental challenge. The high-temperature experiments on iron and iron-nickel alloys at multi-megabar pressure range have still been limited. In particular, the data on iron around 300 GPa that is close to the inner core pressure are available only up to 1350 K [1]. The Fe-Ni alloy was studied up to 255 GPa at room temperature [2] and only to 225 GPa at high temperatures [3]. Note that it is difficult to study the solid-state iron at the inner core pressure by a shock compression method, because the Hugoniot intersects its melting curve at about 250 GPa. Is the  $\beta$ -phase of iron with *dhcp* or orthorhombic structure stable at high *P-T*? How does nickel affect the phase relation of iron? To determine the stable phase relations of iron-nickel alloys at high pressure and high temperature, we conducted laser-heated DAC (LHDAC) experiments on iron and iron-nickel alloys up to 301 GPa and 2000 K.

We have examined six different compositions of iron and iron-nickel alloys: pure Fe, Fe-18.4 wt% Ni, Fe-24.9 wt% Ni, Fe-29.8 wt% Ni, Fe-35.7 wt% Ni, and Fe-50.0 wt% Ni. The chemical compositions and homogeneities of these alloys were examined using

a JEOL JXA-8800 electron microprobe. High-pressure conditions were generated using a symmetric DAC with flat 300  $\mu\text{m}$  culet diamonds for pressures below 90 GPa. We used beveled diamond anvils with 150 and 90  $\mu\text{m}$  culet for pressures up to 180 GPa and 60  $\mu\text{m}$  culet for pressures above 180 GPa. The samples were loaded into a hole drilled in a pre-indented rhenium gasket, together with thermal insulation layers of MgO. In some runs on pure iron,  $\text{SiO}_2$  was used as a pressure medium. After compression to a pressure of interest at room temperature, the sample was heated by a focused TEM<sub>01</sub>\*-mode Nd:yttrium-lithium-fluoride (YLF) laser by double-side heating technique, which minimizes the axial temperature gradient in the sample. High-

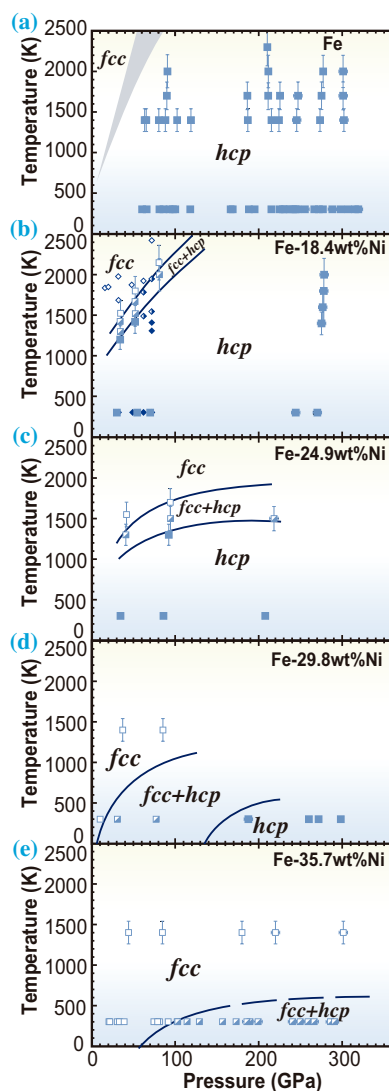


Fig. 1. Phase relations of iron and iron-nickel alloys [4]. Squares: this study; diamonds: previous results for Fe-20 wt.% Ni by Mao *et al.* [6].

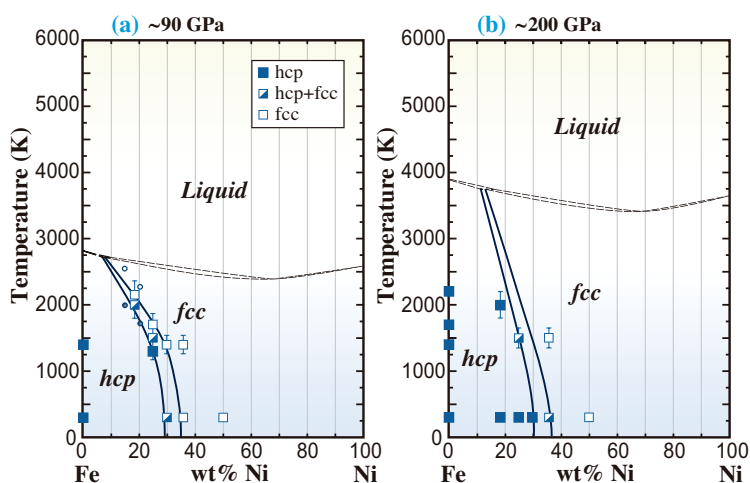


Fig. 2. T-x phase diagrams of iron-nickel alloy at (a) around 90 GPa and (b) 200 GPa [4].

pressure XRD measurements were performed using synchrotron radiation at beamline **BL10XU**. Angle-dispersive XRD patterns were obtained on an imaging plate (Rigaku R-AXIS IV) and X-ray charge-coupled device (CCD) (Bruker APEX).

Experimental results on iron and iron-nickel alloys are summarized in Fig. 1. *In situ* XRD measurements demonstrate the wide stability of *hcp*-iron up to 300 GPa and 2000 K without phase transition to *dhcp*, orthorhombic, or *bcc* phases. Our results also showed that the incorporation of nickel significantly expands the stability field of the *fcc* phase. Figure 2

shows the temperature-composition (*T-x*) phase diagrams of the iron-nickel binary system at around 90 and 200 GPa. In this figure, the composition of the *fcc-hcp-liquid* triple point is important, considering the crystalline phase at the inner core-outer core boundary (ICB). For example, if the nickel content in the outer core is lower than that of the *fcc-hcp-liquid* triple point, the *hcp* phase crystallizes during the inner core crystallization (Fig. 3(a)). In contrast, if the nickel content in the outer core is larger than that of the triple point, the *fcc* phase should crystallize at the ICB (Fig. 3(b)). Furthermore, the *fcc* phase may transform to an *hcp* structure at the deep inner core with Earth's secular cooling (Fig. 3(c)).

According to our results, the *fcc-hcp-liquid* triple point is located at about 8% Ni at 90 GPa and 12% Ni at about 200 GPa. The nickel content in the Earth's core is unclear, but most of the literature suggested 5 to 10% Ni on the basis of the chondritic Earth model [5]. If this is true, the *hcp* phase should crystallize at the ICB.

Although realizing the *P-T* conditions of the center of the Earth (~360 GPa, ~6000 K) in the laboratory requires further technical developments, the novel LH-DAC technology will open up new windows to explore this region of the Earth and deep interiors of other planets.

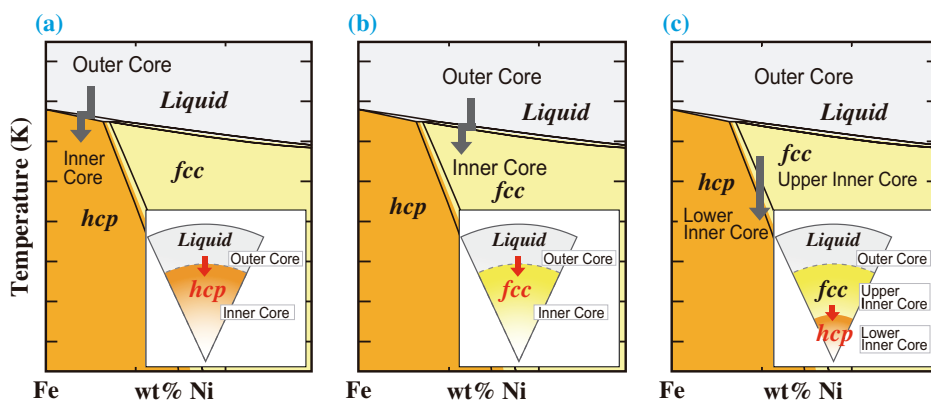


Fig. 3. Schematic phase diagrams of iron-nickel system at the pressure of the inner core boundary. (a) If the Ni content in the outer core is less than that of the *fcc-hcp-liquid* triple point, the inner core could be composed of the *hcp* phase. (b) If the nickel content in the outer core is larger than that of the triple point, the *fcc* phase should first be crystallized at the inner core boundary. (c) The *fcc* phase may transform to the *hcp* structure with secular cooling. Insets, schematic images of the Earth's inner core structure.

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## References

- [1] L.S. Dubrovinsky *et al.*: Phys. Rev. Lett. **84** (2000) 1720.
- [2] H.K. Mao *et al.*: J. Geophys. Res. **95** (1990) 21737.
- [3] L. Dubrovinsky *et al.*: Science **316** (2007) 1880.
- [4] Y. Kuwayama, K. Hirose, N. Sata and Y. Ohishi: Earth Planet. Sci. Lett. **273** (2008) 309.
- [5] W.F. McDonough: Treatise on Geochemistry, Elsevier, Amsterdam, vol. 2, (2004) 547.
- [6] W.L. Mao *et al.*: Phys. Earth Planet. Inter. **155** (2006) 146.