

## **Iron-Nickel Alloy in the Earth's Core**

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### **Abstract**

The phase relations of an Fe10wt%Ni alloy were investigated in a diamond anvil cell up to 86 GPa and 2382 K. Adding nickel into iron stabilizes the fcc phase to higher pressures and lower temperatures compared to pure iron, and a region of two-phase coexistence between fcc and hcp phases is observed. Iron with up to 10 wt% nickel is likely to be in the hcp structure under inner core conditions. The axial ratio ( $c/a$ ) of hcp-Fe10wt%Ni has a weak pressure dependence, but it increases substantially with increasing temperature. The extrapolated  $c/a$  ratio at ~5700 K and ~86 GPa is approximately 1.64, lower than a theoretically predicted value of nearly 1.7 for hcp-Fe at 5700 K and inner-core pressure. A lower  $c/a$  ratio should have an effect on the longitudinal anisotropy of the hcp phase, and hence, may influence the interpretation of the seismic wave anisotropy of the inner core.

## Introduction

Iron-nickel (Fe-Ni) alloy is the most abundant component in the Earth's core (Birch, 1952). The amount of Ni in the core is about 5.5 wt%, based on geochemical models (McDonough and Sun, 1995). Therefore, the high-pressure properties of Fe-Ni alloy are the starting point for understanding the nature of the Earth's core. The phase diagram and physical properties of Fe have been extensively studied (Hemley and Mao, 2001). Iron crystallizes in the body-centered cubic (bcc) structure under ambient conditions, and transforms to hexagonal close-packed (hcp) structure under high pressures and to face-centered cubic (fcc) structure under high temperatures (Shen et al., 1998). hcp-Fe has a wide stability field extending to inner-core conditions (Hemley and Mao, 2001).

The phase diagrams of Fe-Ni alloys were previously investigated in an externally heated diamond anvil cell (EHDAC) by Huang et al. (1988; 1992). Their results suggested that fcc and hcp phases may coexist under inner-core conditions (Huang et al., 1988); if this is correct, it would be important to our understanding of the formation and properties of the inner core. However, the experiments of Huang et al. (1988) were limited to the relatively low pressure-temperature (P-T) range (25 GPa and 873 K) of an EHDAC. Application to core conditions was made difficult by the large extrapolation to higher P-T and by the sluggishness of the hcp-fcc transition at low temperature, which made determination of the phase transition imprecise. Therefore, we studied an Fe10%Ni (in wt%) alloy in a laser-heated diamond anvil cell (LHDAC) and EHDAC in order to examine the alloying effect of Ni on the phase diagram

closer to inner-core conditions. The axial ratios ( $c/a$ ) of hcp-Fe10%Ni and hcp-Fe7.9wt%Si (Lin et al., 2002) were also determined from high P-T x-ray diffraction patterns and compared to that of hcp-Fe in order to understand the effect of Ni and Si on the  $c/a$  ratio of hcp-Fe under high P-T conditions.

## Experiments

The starting material, Fe10wt%Ni ( $\pm 0.5$  wt% Ni) in the bcc structure, was obtained from Prof. William A. Bassett at Cornell University. A thin, flat disk of the sample, approximately 10  $\mu\text{m}$  in thickness and 50  $\mu\text{m}$  in diameter, was loaded into a DAC having a stainless steel sample chamber that was 100  $\mu\text{m}$  in diameter and 25  $\mu\text{m}$  in thickness. A sandwiched sample configuration, using dried NaCl as the thermal insulator and pressure medium, was used in this study (Birch, 1978; Heinz and Jeanloz, 1984; Shen et al., 2001).

A double-sided Nd:YLF laser heating system, operating in multimode ( $\text{TEM}_{00} + \text{TEM}_{01}$ ), was used to laser heat the sample from both sides of a DAC at the GSECARS sector of the Advanced Photon Source (APS), Argonne National Laboratory (ANL) (Shen et al., 2001). The laser beam diameter was about 25  $\mu\text{m}$ . Greybody temperatures were determined by fitting the thermal radiation spectrum between 670 nm and 830 nm to the Planck radiation function (Shen et al., 2001). The temperature uncertainty ( $1\sigma$ ) averaged from multiple temperature measurements and temperatures from both sides of the sample across the laser-heated spots was about 50 to 150 K in most of the experiments. A white beam or a monochromatic beam was

used as the x-ray source, for either energy-dispersive x-ray diffraction (EDXRD) or angle-dispersive x-ray diffraction (ADXRD), respectively. The synchrotron x-ray beam was about 8  $\mu\text{m}$  in diameter. The diffracted x-rays were collected by a germanium detector at a fixed angle ( $2\theta$ ) of about  $8^\circ$  in EDXRD, or by a CCD in ADXRD. Pressures were calculated from the room temperature equation of state of NaCl (Heinz and Jeanloz, 1984; Birch, 1978) before laser heating. No thermal pressure corrections were made to the pressures at high temperatures in LHDAC experiments. The quenched samples from the LHDAC were polished and then analyzed with a scanning electron microprobe (SEM), the JEOL 5800-LV, at the University of Chicago.

An EHDAC was also used to study the phase transitions of Fe10%Ni (Bassett et al., 1993) in ADXRD experiments. The thermal EOS of NaCl in the B1 structure was used as the internal pressure calibrant (Birch, 1986). These experiments involve P-T conditions that are lower but better controlled than the LHDAC experiments.

## Results

The phase relations of an Fe10%Ni alloy were studied in a LHDAC cell from 30 GPa to 86 GPa and from 1200 K to 2382 K and in an EHDAC up to 27 GPa and 1000 K (Figure 1). bcc-Fe10%Ni transformed to the hcp phase under high pressures. Upon heating, hcp-Fe10%Ni transformed to a mixture of fcc+hcp phases under high temperatures, and upon further heating, the fcc+hcp phases transformed to the fcc phase only (Figure 2). The volume of the hcp phase is about 1% smaller than that of the coexisting fcc at approximately 40 GPa and 1602 K. SEM

analyses of the quenched sample from about 42 GPa and 1438 K also show that the Ni concentration in the laser heated area varies from 8.4 to 10.6 wt%, while the Ni concentration remains at about 10.1 wt% ( $\pm 0.5$ ) in the surrounding unheated area, reflecting Ni partitioning between the hcp and fcc phases. The axial ratios ( $c/a$ ) of hcp-Fe10%Ni and hcp-Fe8%Si (Lin et al., 2002) at various P-T were determined (Figure 3).

### **Discussion and Conclusions**

Compared to the phase diagram of pure Fe (Hemley and Mao, 2001), it is evident that the stability field of the fcc phase can be extended to higher pressures and lower temperatures with the addition of Ni (Figure 1). However, the effect of Ni on the phase diagram of Fe is not as dramatic as the addition of silicon in Fe (Lin et al., 2002). Nickel remains in the fcc structure under high pressures (Rekhi et al., 2001), and Fe transforms to the hcp structure under high pressures (Hemley and Mao, 2001). The difference between the phase diagrams of Ni and Fe indicates that a region of two-phase equilibrium should exist between fcc and hcp phases of Fe-Ni alloy under high pressures. A region of two-phase coexistence between fcc and hcp phases is observed under high P-T in this study (Figure 1).

Extrapolating the region of two-phase coexistence to higher P-T conditions, it is seen that Fe with up to 10 wt% Ni is in the hcp structure under inner-core conditions. The slope of hcp to fcc+hcp phase transformation for Fe10%Ni is steeper than that extrapolated from EHDAC experiments on Fe10%Ni (Huang et al., 1988). The amount of Ni in the core is only about 5.5 wt% (McDonough and Sun, 1995). Hence, the crystal structure of the inner core is likely to be

in the hcp structure assuming that Ni is not strongly partitioned into the inner core, and that the inner core only contains a small amount of elements other than Fe (Lin et al., 2002).

The  $c/a$  ratios of the hcp-Fe10%Ni and hcp-Fe8%Si decrease slightly with increasing pressure and increase substantially with increasing temperature (Figure 3). This behavior has been recognized at relatively lower P-T conditions and discussed previously for hcp-Fe (Steinle-Neumann et al., 2001). The extrapolated  $c/a$  ratio at 5700 K from a weighted least-squares linear fit of the data is approximately 1.64 for hcp-Fe10%Ni at ~86 GPa and 1.67 for hcp-Fe8wt%Si at ~76 GPa, lower than a theoretically predicted value of 1.7 for hcp-Fe at 5700 K and inner-core pressure (Steinle-Neumann et al., 2001). The  $c/a$  ratio of hcp-Fe measured experimentally at ~161 GPa and ~2450 K is about 1.605, similar to that measured at lower P-T conditions (Hemley and Mao, 2001) but inconsistent with the theoretical calculations (Steinle-Neumann et al., 2001). More experiments on the  $c/a$  ratio of Fe should be conducted in order to resolve this discrepancy. The x-ray intensity of the hcp (002) diffraction decreases with increasing pressure in ADXRD experiments, indicating that the hcp crystals display preferred orientation (or texture) at high pressures, with the  $c$ -axes parallel to the loading axis of the DAC (Wenk et al., 2000). Nevertheless, according to the data of Wenk et al. (2000), nonhydrostatic effects on the  $c/a$  ratio of hcp-Fe are small even under the extreme conditions of 220 GPa and 300 K. The changes in the elastic constants of hcp-Fe as a consequence of an increasing  $c/a$  ratio (Steinle-Neumann et al., 2001) have been used to explain the seismological observations of the inner-core anisotropy (Tromp, 2001). A lower  $c/a$  ratio would reduce the anisotropy of the hcp phase

(Steinle-Neumann et al., 2001), which may influence the interpretation of the seismologically observed anisotropy of the inner core.

### **Acknowledgments**

We thank GSECARS at APS, ANL for providing the synchrotron beamtime and the William M. Keck Foundation for funding the facility. We also thank W. Bassett, A. Davis, I. Steele, V. Prakapenka, G. Steinle-Neumann, E. Huang, and F. Li for their assistance. This research is supported by NSF grant EAR-9974373 to D.L.H. and NASA grant NAG5-9800 to M. Humayun.

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**Figure Captions:**

**Figure 1.** Phases observed in LHDAC and EHDAC experiments with a starting material of Fe10%Ni. Black lines: the phase diagram of iron (Hemley and Mao, 2001); thick grey lines: limits of fcc+hcp phase region in Fe10%Ni.

**Figure 2.** Representative ADXRD patterns of Fe10%Ni at 40 GPa in a LHDAC. A monochromatic beam (wavelength = 0.4066 Å) was used as the x-ray source. Diffraction peaks from hcp, fcc, and B2-NaCl (pressure calibrant) phases are labeled.

**Figure 3.** Axial ratios ( $c/a$ ) of hcp-Fe10%Ni and hcp-Fe8%Si (Lin et al., 2002) above 68 GPa as a function of temperature. Standard deviation of the  $c/a$  ratio is approximately 0.005. Typical error bar on temperature and  $c/a$  ratio is shown in the lower right-hand corner. Theoretical calculation for hcp-Fe at constant volume: Steinle-Neumann et al., 2001; experimental result for hcp-Fe: Hemley and Mao, 2001.



Angle-dispersive x-ray patterns at 40 GPa

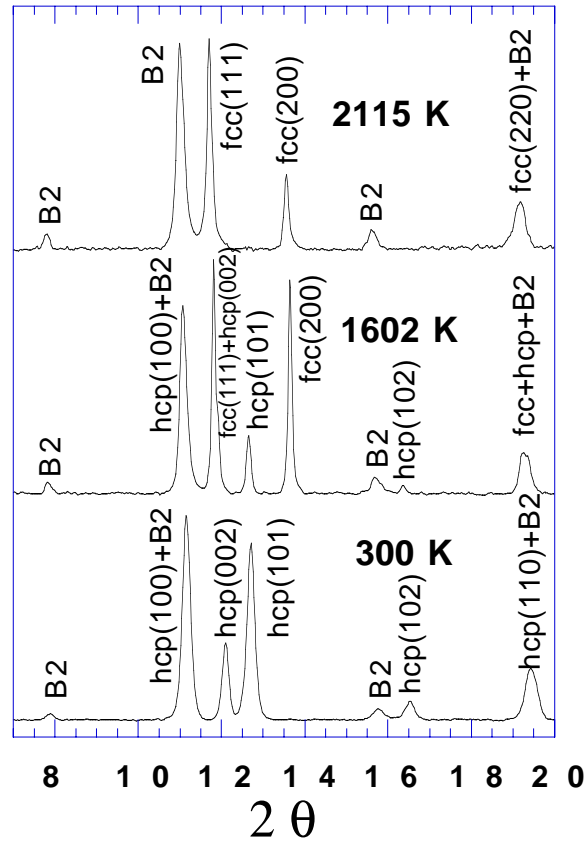


Figure 2

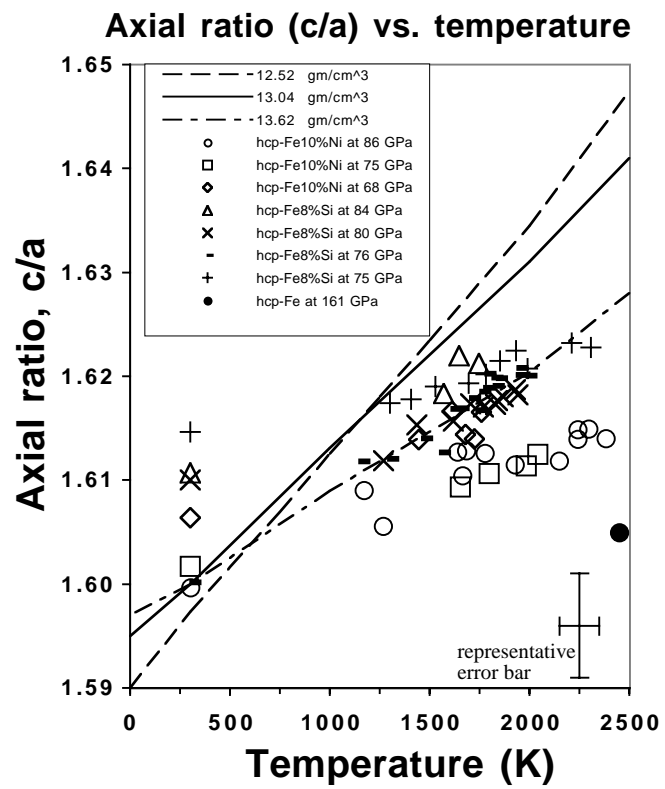


Figure 3