Structure of iron in Earth's inner core

The inner core, the most remote part of our planet, is composed of solid iron. A number of observations show anisotropy in seismic wave speed, which is most likely caused by the preferred orientation of iron. The crystal structure in the inner core provides key information for deciphering such observations and understanding the inner core dynamics. Owing to limited accessibility in an ultrahigh pressure and temperature (*P-T*) experiment to the real conditions of the inner core (reaching >330 GPa and ≥5000 K), the crystal structure of iron at the inner core has long been under debate.

Iron adopts a body-centered-cubic (*bcc*) structure under ambient condition and transforms into the hexagonal close-packed (*hcp*) phase above 15 GPa. While *hcp*-Fe can persist to core pressures at 300 K [1], a phase transition at elevated temperature is a possibility. Both theory and experiments proposed different forms of iron at simultaneously high *P-T* conditions, which include *bcc*, face-centered-cubic (*fcc*), and *hcp* structures. The structure of iron has never been examined experimentally under the inner core *P-T* conditions, because such extreme conditions could only be achieved by dynamical shock-wave experiments on a microsecond order. On the basis of a combination of static compression experiments in a laser-heated diamond-anvil cell (DAC) and synchrotron X-ray diffraction (XRD) measurements, we first determined that the hexagonal *hcp* structure is a stable form of iron up to 377 GPa and 5700 K, corresponding to inner core conditions [2].

Angle-dispersive X-ray diffraction (XRD) measurements were conducted at the dedicated beamline **BL10XU**, for high-pressure research. The XRD patterns were collected *in situ* at high *P-T* on a CCD detector (Bruker APEX) with a typical exposure time of 10 sec. A monochromatic incident X-ray beam was focused by stacked compound refractive lenses (CRLs) and collimated to about 6 μm (full width at half maximum) in diameter on the sample. For experiments beyond 300 GPa, double-beveled diamond anvils with 40 μm culets were used, and accordingly, the sample size was limited to about 20 μm. Heating was performed from both sides of the sample by employing a couple of 100 W single-mode Yb fiber lasers (SPI). We used beam shaping optics, which converts a Gaussian beam to one with a flatter energy distribution in an attempt to reduce the radial temperature gradient in the sample. The laser-heated spot was ~15 μm across. Temperature was measured by the spectroradiometric method.

To construct the phase diagram of iron to core conditions, we conducted six separate sets of experiments. The first experiment at 303 GPa and room temperature resulted in an XRD pattern that included peaks from *hcp*-Fe and Re (gasket material). Subsequently, we heated this sample to 4820 K at 332 GPa (Fig. 1(a)). The one-dimensional XRD pattern did not change except the appearance of the *hcp* 002 line. On the other hand, the two-dimensional image became spotty, indicating crystal growth, and hence, the stability of *hcp*-Fe under these *P-T* conditions. Following these measurements, the sample was temperature-quenched and then further compressed to 321 GPa at room temperature. We again heated the sample to 5520 K at 356 GPa. The XRD pattern was still dominated by the *hcp* phase, but minor peaks assigned to pyrite-type SiO_2 (pressure medium) and Fe_3C cementite appeared (Fig. 1(b)). The measured lattice parameters and

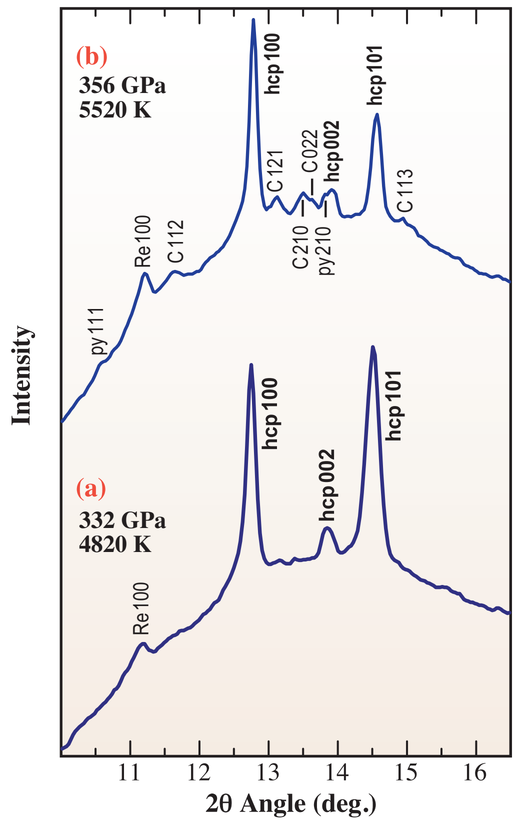

Fig. 1. Representative XRD patterns of *hcp*-Fe at **(a)** 332 GPa and 4820 K and at **(b)** 356 GPa and 5520 K. Labels indicate *hcp*, *hcp*-iron; py, pyrite-type SiO_2 (pressure medium); C, Fe_3C cementite; Re, rhenium (gasket).

volumes of Fe_3C are in agreement with earlier experimental results to 187 GPa. Similar observations were made in five other experiments, which were conducted in a wide *P-T* range from 135 GPa and 2690 K to 377 GPa and 5700 K. In all the measurements, we obtained no evidence of a phase transition to *bcc* or *fcc* iron phases.

These results indicate that *hcp* is a stable form of iron up to 377 GPa and 5700 K, compatible with previous *ab initio* calculations (Fig. 2). The estimation of temperature at the inner-outer core boundary ranges from 4850 to 5700 K, depending on the melting temperature of iron and the effect of light alloying elements. The temperature gradient should be very small within the inner core. Our experiments thus represent the range of inner core *P-T* conditions. One limitation of these experiments is that chemical impurities such as silicon and sulfur, which have the ability to change the stable crystal structure, were not accounted for.

Strong seismic anisotropy exists in the inner core, with longitudinal waves traveling ~3% faster along the polar axis than in the equatorial plane. This was originally attributed to the preferred orientation of *hcp*-Fe, which exhibits a strong single-crystal elastic anisotropy, at least, at low temperature. However, recent calculations [3,4] reported that the *c/a* ratio approaches the value of 1.6299 for the ideal *hcp* structure at high temperature, and consequently, elastic anisotropy of *hcp*-Fe no longer exists under inner core conditions (Fig. 3). On the other hand, experimental evidence previously suggested a weak temperature dependence of the *c/a* ratio at 140 GPa [5], as do our data at ~330 GPa. The *c/a* ratio of 1.602 at 332 GPa and 4820 K, which is substantially lower than the ideal value, suggests that *hcp*-Fe should be elastically anisotropic even under the high temperature conditions of the inner core. The observed seismic anisotropy may therefore result from the preferred orientation of the *hcp* phase with the *c*-axis parallel the Earth's rotation axis.

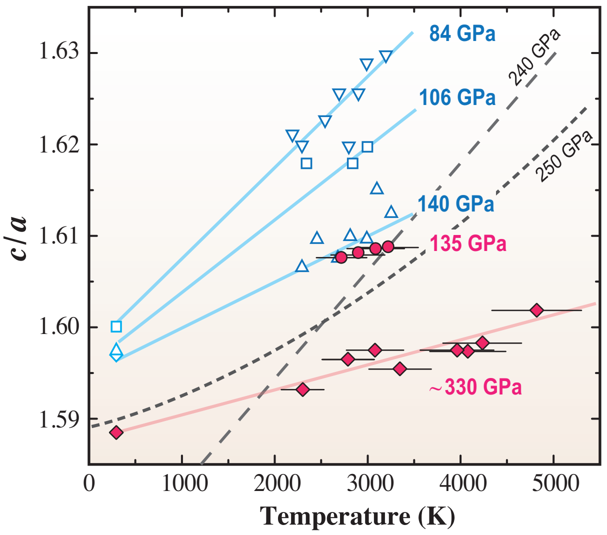

Fig. 3. Temperature dependence of the *c/a* axial ratio of *hcp*-Fe collected at 135 GPa and ~330 GPa (red). The results of theoretical calculations are also shown by a dashed curve [3] and a dotted curve [4]. Previous experimental results at 84, 106, and 140 GPa are from Boehler *et al.* [5] (blue).

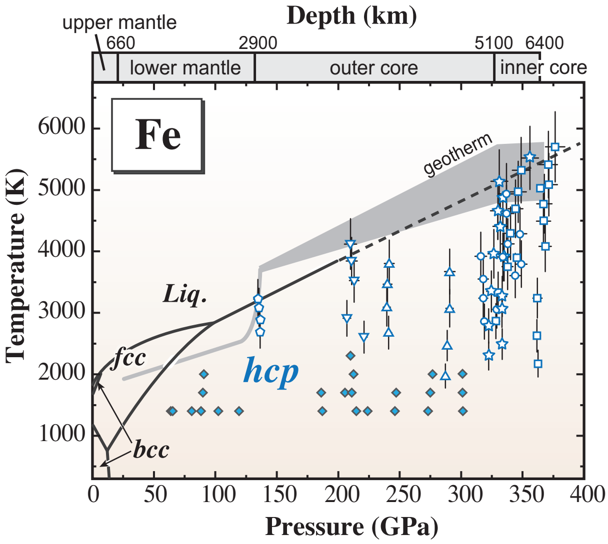

Fig. 2. Phase diagram of iron and the inferred temperature profile inside the Earth. Open symbols indicate present results, and filled diamonds are from previous experimental work [1].

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