

Phase transition in FeO and its implications for two-layered convection in Earth's outer core

Earth's core resides in the center of our planet and constitutes one-sixth of the planet's volume and one-third of its mass. At a depth of 5150 km, the core is divided into two parts, a solid inner core and a molten outer core (Fig. 1). The Earth's liquid outer core includes substantial amounts of light elements in addition to iron and nickel. As the Earth cools, the solid core grows by crystallizing from the liquid core. The latent heat of fusion and chemical buoyancy arising from the exclusion of light elements from the inner core, which are released at the inner-core boundary, drive the outer core convection responsible for dynamo action and thus the Earth's magnetic field. The existence of oxygen as a light element in the core has been put forward to account for the observed seismic-wave velocities and the density jump at the inner core boundary. The structures of light element-bearing phases in the outer core conditions not only impart density variation, but may also influence the geodynamic processes that are controlled by core convection. Iron monoxide (FeO), the major oxygen-bearing phase, adopts the sodium chloride-type (B1) structure under ambient conditions and the nickel arsenide-type (B8) structure under high pressure [1,2] (Fig. 2); however, phase relations under high-pressure and -temperature (P - T) conditions of the outer core are unknown.

All the high P - T experiments were conducted at beamline **BL10XU**. The high P - T conditions were generated in a laser-heated diamond-anvil cell using double-beveled anvils with a 40 μm culet. We prepared the starting material by mixing the powders of $\text{Fe}_{0.96}\text{O}$ and metallic iron. The sample mixture was loaded

into a hole in a pre-indented rhenium gasket, together with thermal insulation layers of SiO_2 glass. The samples were heated by a couple of 100 W single-mode Yb fiber lasers by the double-side heating technique. The laser-heated spot was $\sim 15\ \mu\text{m}$ in diameter. Temperature was measured by the spectroradiometric method. Angle-dispersive X-ray diffraction (XRD) spectra were collected on a charge coupled device or an imaging plate detector with typical exposure times of 10 s and 3 min, respectively. A monochromatic incident X-ray beam with a wavelength of $0.41388\text{--}0.42387\ \text{\AA}$ was collimated to about a $6\text{-}\mu\text{m}$ area (full-width of half maximum) on the sample.

Two separate sets of experiments were conducted at pressures between 227 and 324 GPa and temperatures up to 4880 K [3] (Fig. 2). In the first run, the sample was initially compressed to 266 GPa and subsequently heated. We observed the diffraction peaks only from hexagonal-close-packed (hcp) iron and rhenium before heating and then those from B8 FeO during heating to 2430 K. After a pressure increment at room temperature (Fig. 3(a)) and reheating to 3170 K at 305 GPa, new peaks, which are assigned to 100 and 110 lines of the cesium chloride-type (B2) structure, appeared in the diffraction patterns. During additional heating at 2990 to 4180 K, these B2 peaks became more intense (Fig. 3(b)), indicating the stability of B2 FeO under these P - T conditions. Similarly, in the second set of experiments, B8 FeO was first synthesized at 287 GPa and 2400 K. The B2 phase appeared with increasing temperature to 4100 K at 311 GPa, whereas the diffraction from the B8 phase became weaker. Additional heating cycles were then performed with decreasing/increasing pressure. Whereas only the broad diffraction peaks from B2 FeO and rhenium (gasket) were found after decompression to ~ 210 GPa at 300 K, we observed the B8 phase upon heating to 3400 K and subsequently the B1 phase above 3690 K at 230 GPa.

These results indicate that the B2 phase of FeO is stable above 230 GPa along the melting curve (Fig. 2). B1 FeO transforms directly to B2 above 3850 K. The volume change across the B1-B2 transition is 1.9%, on the basis of the volumes of B1, B2, and B8 phases (11.901 , 11.679 , and $11.815\ \text{\AA}^3$ per formula unit, respectively) coexisting in the XRD pattern collected at 230 GPa and 3690 K near the triple point. While the B1/B2 phase transition boundary is not tightly constrained in the present experiments, its Clapeyron slope is calculated to

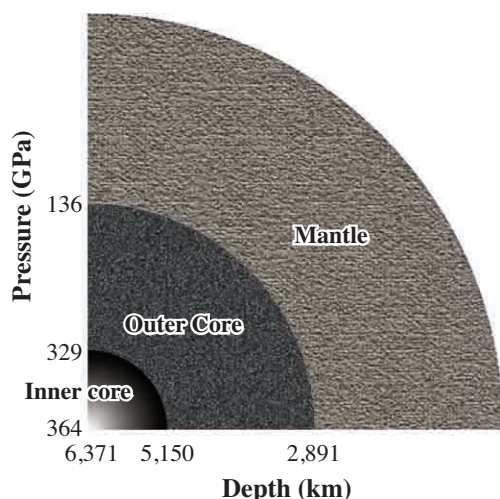


Fig. 1. Cross section of the Earth.

be -6.2 MPa/K from those of B1/B8 and B2/B8 boundaries (-50 MPa/K) and the volume differences between these three phases described above. The negative slope of the B1/B2 boundary is consistent with the fact that the nearest Fe–O bond becomes longer and weaker across the transition owing to an increase in the coordination number from six to eight. Since the volume change is relatively small, this results in smaller vibrational frequencies overall and thus higher entropy for the high-pressure B2 phase.

As in crystalline FeO, the structure of liquid FeO would change from a B1- to B2-like arrangement in a comparable or slightly lower pressure range as suggested by previous studies on liquid alkali halides. The oxygen-bearing core liquid would thus change its Fe–O local structure with an increase in the mean coordination number from six to eight at around 240 GPa in the middle of the outer core (Fig. 2). The resulting density increase may be as much as 0.6%, considering the maximum abundance of oxygen in the outer core (~ 20 atm%). According to the numerical simulations, such a density increase and negative Clapeyron slope of the structural boundary suppress the convection, resulting in two-layered convection in the Earth's outer core [3]. The two-layered structure of core convection offers an alternative explanation for the flux patches that characterize Earth's magnetic

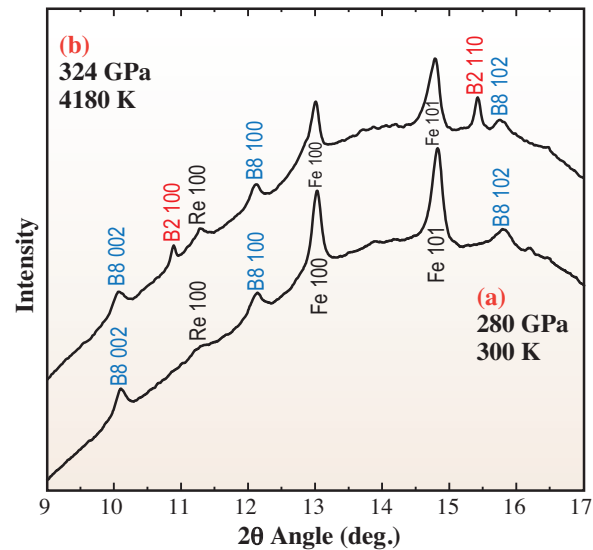


Fig. 3. XRD patterns obtained at (a) 280 GPa and 300 K and (b) 324 GPa and 4180 K in run 1. Fe, hcp-iron; Re, rhenium (gasket).

field. If flows in the upper and lower layers generate magnetic fields with opposite polarities in isolation, reversed patches may be a manifestation of a two-layer dynamo. Such a situation is possible only if the upper and lower dynamos behave independently as a result of strong stratification. Sudden mixing of the upper and lower regions, induced by magnetic and/or kinematic instabilities, may act as a trigger of geomagnetic polarity reversal, because dipole field collapse and subsequent polarity reversal are probably consequences of vigorous convective mixing of the core fluid.

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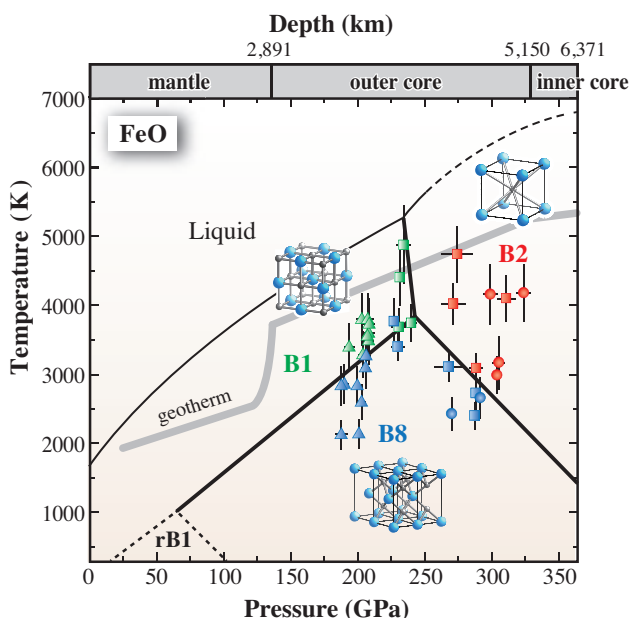


Fig. 2. Phase diagram of FeO. Green, red, and blue symbols represent the stabilities of B1, B2, and B8 structures, respectively. Circles, run 1; squares, run 2; triangles, Ozawa *et al.* [2]. Stability of rhombohedrally distorted B1 (rB1) phase is from Fei and Mao [1]. Melting curve of B1 FeO is from previous experimental work [4]. Crystal structures are also shown: oxygen atoms are represented by blue spheres and iron atoms by gray spheres. The inferred temperature profile inside Earth is shown by gray line.

References

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