

HIGH PRESSURE AND HIGH TEMPERATURE PHASE TRANSITIONS OF FeO

FeO is one of the most abundant oxide components in Earth’s mantle and is also likely incorporated in the core. FeO crystallizes with the NaCl-type structure (B1) under ambient conditions and transforms to a rhombohedral phase above 17 GPa at 300 K [1]. The resistance-heated diamond anvil cell (DAC) experiments showed the transition from rhombohedral to NiAs-type (B8) structure above 90 GPa at 600 K [2]. Fei and Mao [2] further suggested the transition from the B1 to the B8 structure around 70 GPa at high temperature (>1000 K) to be consistent with earlier shock compression studies [3] and electrical resistance measurements [4]. This B1 to B8 transition has never been confirmed at high temperatures.

High-pressure and high-temperature experiments were performed at beamline **BL10XU** using DAC coupled with heating by a Nd:YAG laser [5]. We collected X-ray diffraction patterns of the sample at *in situ* high pressure and temperature conditions up

to 87 GPa and 1730 K. A fine powder of Fe_{0.954}O mixed with Fe (2:1 by mole ratio) was used as a starting material. It was loaded into a 100-μm hole drilled in a rhenium gasket preindented to a thickness of 50 μm, together with a pressure medium of Al₂O₃ polycrystalline pellets. The size of the heating spot was more than 50 μm. The X-ray diffraction data were collected from an area 20 μm in diameter. Exposure times were one to five minutes.

We observed a transition from the B1 to the B8 structure above 70 GPa at 1600 K (Fig. 1). The typical diffraction patterns of FeO with either the B1 or B8 structure are shown in Fig. 2. The relative intensities of diffraction peaks of the B8 structure may indicate the metallic polytype NiAs structure, which is a mixture of inverse (O at Ni site) and normal structures (Fe at Ni site), as proposed by Mazin *et al.* [6]. The metallic features of the polytype NiAs can explain the metallization of FeO

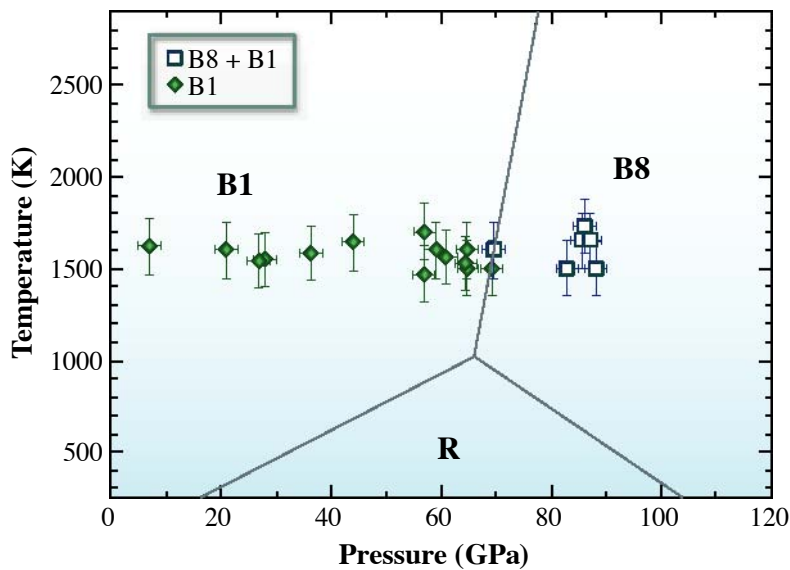


Fig. 1. Phase diagram of FeO. The B1-R and R-B8 transition boundaries are from Fei and Mao [2]. B1, NaCl-type; B8, NiAs-type; R, rhombohedral structure.

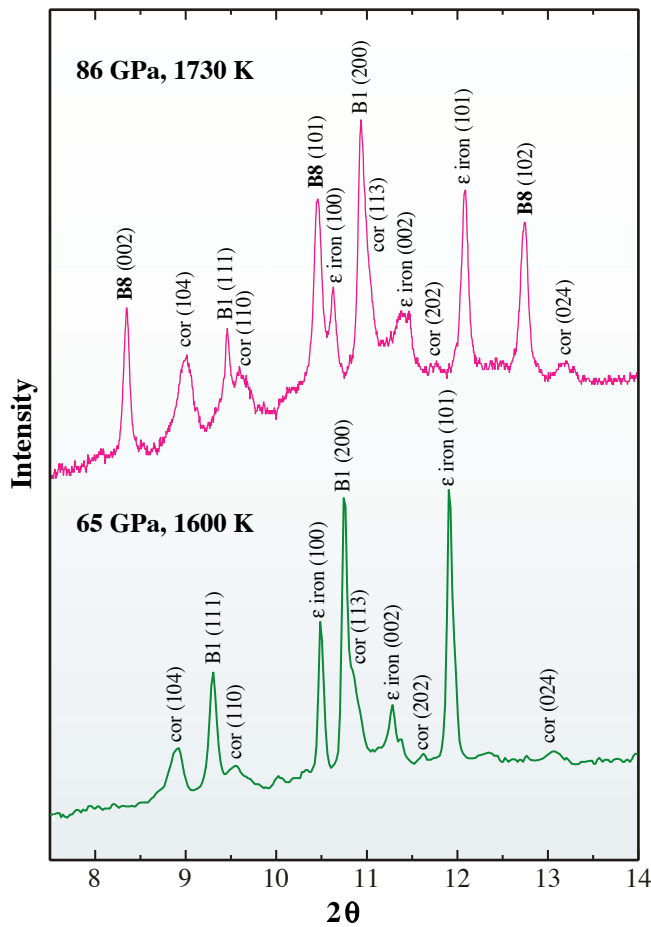


Fig. 2. Examples of X-ray diffraction patterns showing the B1 and B8 structures of FeO together with ϵ -Fe and corundum.

inferred from the resistance measurements [4]. The transition to a metallic phase of FeO could enhance oxygen solubility in molten iron. A structural difference between the B1 structure of MgO and the B8 structure of FeO could lead to an immiscibility gap in the MgO-FeO solid solution above 70 GPa. The lowermost mantle could be enriched with FeO as a result of chemical reactions between silicate perovskite and liquid iron. The FeO-rich (Mg,Fe)O phase with the B8 structure is likely to be present together with MgO-rich ferropericlasite in the deep lower mantle. The presence of the B8 phase should increase the electrical and thermal conductivity, which may explain the nature of a highly electrically conductive layer observed at the bottom 200 m of the Earth's mantle.

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