I075-002 Room: IC Time: May 27 13:45-14:00

High pressure and high temperature phase of FeO

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From seismic observations and high-pressure experiments, the density of the outer core is supposed to be about 10% lighter than molten pure iron (e.g. Birch 1963). Therefore, light elements are generally assumed to exist in the outer core. Among them, oxygen is one candidate, because of its high abundance in solar system (e.g. Ringwood 1977). Since oxygen has very limited miscibility into molten iron at ambient pressure, understanding the miscibility under high pressure is important for oxygen as a candidate of light elements. In addition, the knowledge is also crucial for the core-mantle boundary where the molten outer core contacts the underlying oxides/silicates.

The high-pressure phase of FeO has been supposed to be metallic and enhance the solubility of oxygen into iron. The structure of the high-pressure phase was observed in an external heated diamond anvil cell (Fei and Mao 1994). They assigned the observed phase as the normal B8 phase. However Mazin et al. (1998) interpreted the same x-ray diffraction pattern as a stacking of the normal and inverse B8 phases. In addition, theoretical calculations showed the inverse B8 is more stable than the normal B8 phase in the ground state (e.g. Fang et al. 1999). The inverse B8 phase is predicted to be insulator, while the normal B8 phase to be metallic (Mazin et al. 1998). It is important to clarify the structure.

We have conducted high P-T experiments for non-stoichiometric $Fe_{0.91}O$ with a laser heated diamond anvil cell. X-ray diffraction experiments with an angle dispersive technique were taken at the GeoSoilEnviroCARS beamline (13-ID-D) at the Advanced Photon Source (Shen et al. 2001). We used a stainless guided boron gasket for maintaining sample and insulator thickness. In an isothermal compression at 1500+/-150 K, $Fe_{0.91}O$ was found to transform from the B1 (rock salt structure) to the B8 (NiAs structure) phase at 137+/-5 GPa. The back transformation from the B8 to B1 phase was found at 123+/-6 GPa upon decreasing pressure.

To clarify whether the high P-T phase is the normal B8 or inverse B8 phase, we used the GSAS and EXPGUI program to analyze our observed data at 137 GPa and 1500 K. Figure shows the observed data and the fit with the normal B8 phase. The residual without background (Rwp) was 0.0277. For the inverse B8 phase, the Rwp is more than two times larger (0.0651) than that of the normal B8 phase. This strongly suggests that the observed high-pressure phase has the normal B8 structure.

In the shock wave experiments (e.g. Jeanloz and Ahrens 1980), a density discontinuity started from 70 GPa and finished at 100 GPa. The discontinuity was attributed to the B1-B8 phase transition (e.g. Fei and Mao 1994). However, the transition pressure is different by more than 40 GPa from the result of our study. This large discrepancy in the transition pressure cannot be explained by experimental errors in pressure and temperature measurements. Therefore, our study does not support this interpretation.

Experiments are still in progress for the transition boundary and the possible non-stoichiometric effects. The results will be discussed.

This work is collaborated with Guoyin Shen, Mark L. Rivers, and Stephen R. Sutton (Consortium for Advanced Radiation Sources, University of Chicago)

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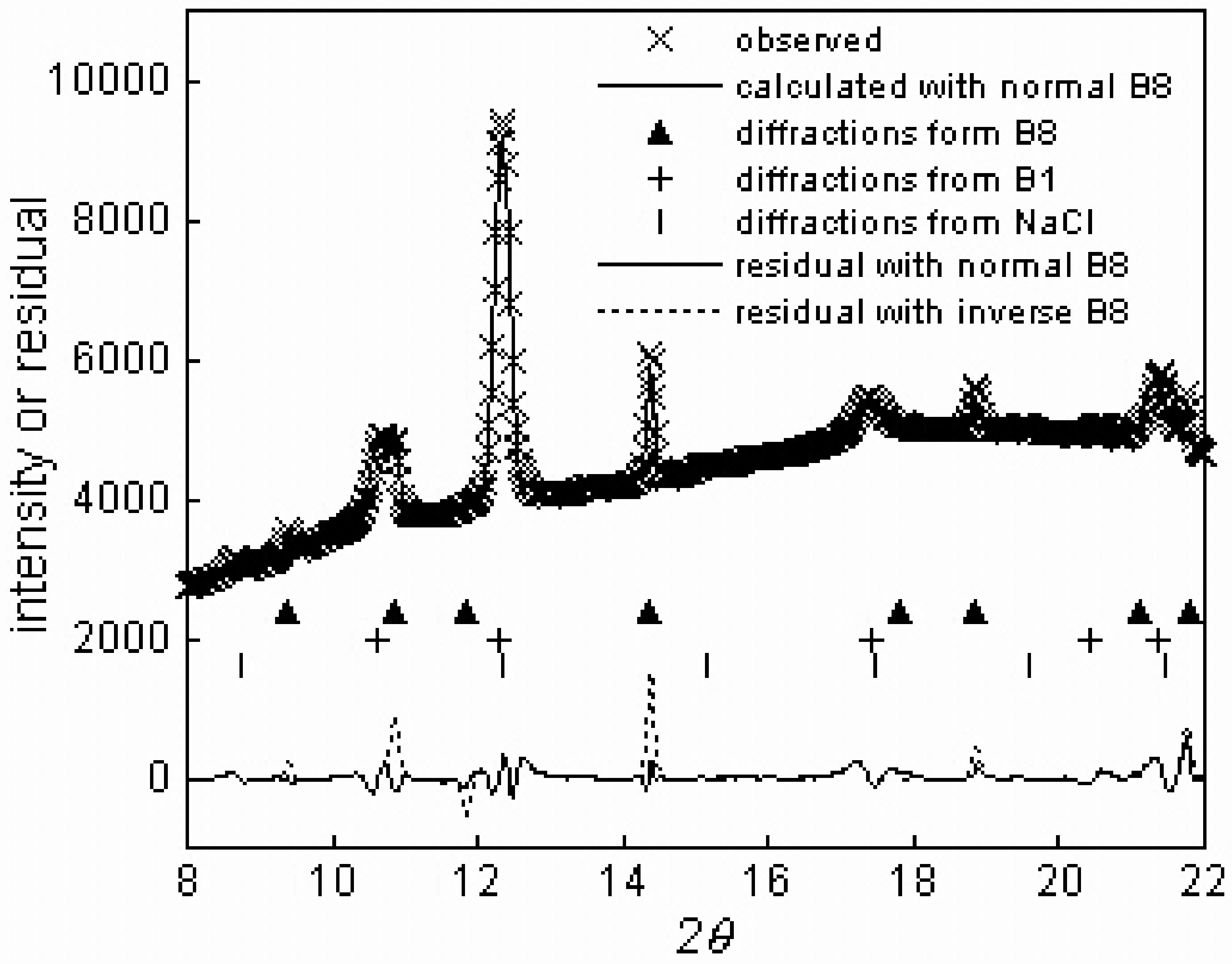

The integrated 1D pattern ($\lambda = 0.4066$ A) from x-ray diffraction for $Fe_{0.91}O$ at 137 GPa and 1500 K. The GSAS and EXPGUI were used for fitting. If the inverse B8 phase is assumed instead of the normal B8 phase, the residual is larger at every diffraction lines of the B8 phase.