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High-pressure structural analysis of Fe_3O_4

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Recently, Todo et al. reexamined pressure effects on the insulator-metal transition (so-called Vervey transition) of Fe_3O_4 with a high quality single crystal. Fe_3O_4 belongs to the inverse spinels, and hence the B site cations take either trivalent (Fe^{3+}) or divalent (Fe^{2+}) state. With decreases of temperature below T_V (= 120 K), Fe_3O_4 shows a sharp insulator-metal transition. They found that the transition disappears above P_c (= 7.5 GPa) and the system remains metallic down to the lowest temperature. This observation will shed a light on the nature of the Vervey transition, which is still controversial. In order to deeply understand the high-pressure effect on the Vervey transition of Fe_3O_4, detailed structural information including the atomic coordinates is indispensable, because hybridization between the Fe3d and O2p orbitals plays an importance role on this transition

High-pressure x-ray powder diffraction were performed at **SPring-8, BL10XU** beamline at room temperature using a specially designed diamond anvil cell (DAC). Precipitation method was adopted in order to get fine and homogeneous powders. Melt-grown crystal ingots were crushed into fine powder and were sealed in a gasket hole of the DAC, 80 micrometer in thickness and 260 micrometer in diameter, which was filled with ethanol/methanol mixture as a pressure-transmitting medium. The Debye-Scherrer powder rings give a homogeneous intensity distribution, which is the necessary condition for a reliable Rietveld analysis. Magnitude of the applied pressure were monitored by the energy of the luminescence line R_1 from a small piece of ruby placed in the gasket hole. The wavelength of the incident x-ray is 0.49547 A and 0.49493 A, and the exposure time was for 10 min. We have analyzed thus obtained x-ray patterns with RIETAN2000 program. (Fig.1) The crystal symmetry remains cubic (Fd3m; Z = 8) in the pressure range up to 20 GPa.

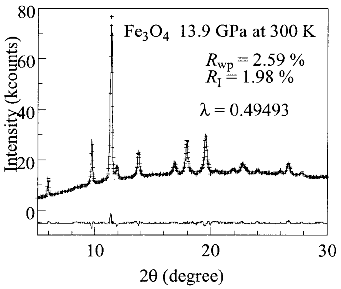

Fig.1: X-ray powder diffraction patterns (cross) of Fe_3O_4 at 13.9 GPa. Solid curve is the results of the Rietveld refinement with inverse spinel (Fd3m; Z = 8) structure.

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Possibility of a reaction between $MgCO_3$ and iron under the lower mantle conditions

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$MgCO_3$ magnesite is considered to be stable in the lower mantle and one of important minerals on transportation of light elements into Earth's outer core. It was suggested that the reaction between $MgCO_3$ and iron in the lower mantle occurs and the Fe_3C could transport carbon during core formation. ($MgCO_3 + 5Fe \rightarrow Fe_3C + MgO + 2FeO$) [1] In this work, we tried to evaluate the possibility of this reaction under the lower mantle conditions using a laser-heated diamond anvil cell.

The sample was natural magnesite powder with a small amount of iron powder. Al_2O_3 powder was used as a thermal insulator between the sample and the diamond. A pre-indented Rhenium gasket was used and sample chamber was about 150 μm in diameter. A conventional ruby fluorescence method was used for determining sample pressure. Nd-YAG(150W) laser was used and the size of a hot spot in the sample chamber was about 50 μm in diameter. Experiment was carried out at the condition of 42GPa and 1500K. X-ray beam was monochromatized to the wavelength of 0.4133 Å and was collimated to 20 μm in diameter.

Figure 1 shows the observed diffraction peaks. We found some new diffraction peaks at 42GPa and 1500K. It is still controversial that these new peaks come from some reaction products. Further studies of assignment of new diffraction peaks are now in progress.

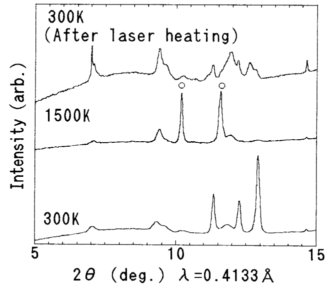

Fig.1 Observed diffraction patterns. Open circles represent new peaks.

[1] H.P.Scott, Q.Williams & E.Knittle, Geophys. Res. Lett., 28(9), 1875-1879, 2001