Pressure-induced phase transition of Fe3-xTixO4 solid solution

Tetsurou Mine[1]; Taku Okada[2]; Takamitsu Yamanaka[3]; Takaya Nagai[4]

[1] Earth and Space Sci., Osaka Univ; [2] Dep. Earth and Space Sci., Osaka Univ. ; [3] Dept. Earth and Space Osaka Univ.; [4] Earth and Planetary Sciences, Hokkaido Univ.

http://globe3.ess.sci.osaka-u.ac.jp/

Introduction Titanomagnetites Fe3-xTixO4,the solid solution between Fe3O4 and Fe2TiO4, have an inverse spinel structure (space group Fd-3m,Z=8)with a mixed valence iron. Ti4+ ions exclusively occupy octahedral (B) sites and Fe2+ and Fe3+ ions occupy both tetrahedral (A) sites and octahedral (B) sites. The high-pressure studying of titanomagnetites, which are the most abundant mineral responsible for magnetic and electric properties in crust, is crucial for geophysics. Also magnetite Fe3O4, end-member in the solid solution, is interested in the technological applications and extensively investigated because of ferrimagnetism and electric conduction by electron hopping. And it is suggested that magnetite transforms into high-pressure phase (h-Fe3O4 phase) with CaMn2O4-type (Pbcm) or CaTi2O4-type (Bbmm) at 24.2GPa and 823K , and at 24.0GPa and ambient temperature (Fei et al., 1999; Haavik et al., 2000).

In this study, we performed high-pressure X-ray powder diffraction measurements at ambient temperature for titanomagnetites with x=0.1, 0.25, 1.0 and investigated the dependence of composition(x) and pressure in their structure and behavior.

Experimental To synthesize the starting materials the required quantities of Fe2O3 and TiO2 powders were sintered at 1450C in an Ar atmosphere. The spinel structure and uniformity of composition was verified by X-ray powder diffraction and SEM-EDS, respectively. The high-pressure experiments were carried out using lever type diamond anvil cell (DAC) at KEK BL13A and BL18C at ambient temperature. The powdered titanomagnetites sample and pressure-transmitting media of 16:3:1 methanol:ethanol:H2O mixture was compacted in a sample chamber, drilled in a preindented Re gasket. Pressure was determined from ruby fluorescence.

Result and Discussion In the diffraction data of the sample with x=1.0, a new diffraction peak appeared at 8GPa. This indicate phase transition from cubic to tetragonal structure. This transition occurs probably at the lowest pressure in that of other spinels. In addition, another peak appeared at 15GPa, while peaks of tetragonal structure phase completely disappeared at 22GPa. Another new phase can be described as high-pressure phase of magnetite (h-Fe3O4) by comparing two diffraction patterns.

In the diffraction data of the sample with x=0.25, a new diffraction peak appeared at 22GPa This phase was not tetragonal phase, but h-Fe3O4 phase. After additional compression, at 42GPa spinel phase remained at h-Fe3O4 phase.

In the diffraction data of the sample with x=0.1, a new diffraction peak appeared at 29GPa. This phase was also h-Fe3O4 phase, and spinel phase remained even at 60GPa. This coexisting phase returned to spinel structure completely at ambient pressure in decompression.

These phases were analyzed for detail structure and the argument in Fe3O4 – Fe2TiO4 system was performed.