High-pressure single crystal diffraction study of MgSiO3 ilmenite and stability of crystal structure

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A high-pressure single-crystal X-ray diffraction study of MgSiO3 ilmenite was carried up to 8.0GPa. The determined isothermal bulk modulus were K0=190(2)GPa(K0'=4 fix) and axial compressibility is anisotropic like other compound of ilmenite structure.MgO6 octahedron is more compressible than SiO6 octahedron. In addition, cation-cation distance becomes shorter along c, in particular the Mg-Si distance across the shared face and Si-Si distance across the vacant site,than between adjacent site across the shared edges. On the other hand, Mg-Mg distance across the vacant site is less compressible. It is interesting for understanding of the structure of MgSiO3 ilmenite under high-pressure stable field.

1) Introduction

Polymorphs of magnesium silicate are generally considered to be an important constituent of the Earth's mantle . MgSiO3-ilmenite is stable in a narrow pressure range of 21 to 25 GPa at 1100 degree(Ito and Yamada 1982). Because of its narrow stability field, MgSiO3-ilmenite is potentially important in a cold (subduction) environment in the transition zone and upper most part the lower mantle.

The ilmenite structure is a nearly hexagonal close packed oxygen array. Layers of edge-sharing octahedral cation sites extend in the (0001) plane. In addition to sharing three edges with other octahedral cations of the same type in the same layer, each cation shares one octahedral face with a cation of the other type in adjacent layer and shares the face opposite to this with a vacant octahedral position. On either side of each vacant octahedral position along c shares cations of the same type.

It is consider the narrow stability field of ilmenite is derived from its crystal structure.The present study was undertaken to characterize the changes in the crystal structure of MgSiO3- ilmenite under compression by high pressure single crystal X-ray diffraction study.

2) Experiment

The single crystal of MgSiO3-ilmenite was synthesized at approximately 22GPa and 1700 degree with run time of 30 minutes, using a uniaxial split sphere apparatus installed at the Institute for study of the Earth's interior. Synthetic orthoenstatite was used as the starting material. The crystal was mounted in a diamond anvil cell (DAC) with a spring steel gasket(260-micron diameter hole and 200-micron thickness).

The pressure-transmitting medium was a 16:3:1 mixture of methanol:ethanol:water. Pressure was calibrated by measuring the shift of the R1 ruby fluorescence line. At the high-pressure condition X-ray intensity data were collected up to 8.0 GPa,using a Four-Circle diffractometer of BL-10A at the Photon Factory.

Refinement was carried out about scale factor, atomic coordinates, isotropic temperature factor and extinction parameter, with full matrix least-squares program RADY89(Sasaki 1989). Corrections were made for Lorentz effect and absorption by the components of the DAC. No absorption corrections of crystal were made because of the small value of ur(<0.1).

3) Result and Discussion

The volume compression data were used for the fitting to a Birch-Murnaghan equation of state. The determined isothermal bulk modulus were K0=190(2) GPa (K0'=4 fix). This is a little smaller than the other results, K0=212GPa obtained by Brillouin scattering(Weidner and Ito 1985) and K0=224GPa(K0'=4.18) obtained by LDA computation(Karki et al 2000). Axial compressibility is anisotropic with Ba=1.30(8) and Bc=2.2(1)(10-3/GPa),like other compounds having ilmenite structure.

The R-value and wR-value were reduced to 4.2% and 4.8% from the result of structural refinement of 4.5 GPa. MgO6 octahedron is more compressible than SiO6 octahedron. In addition, cation-cation distance is greatly shortened along c, in particular the Mg-Si distance across the shared face and Si-Si distance across the vacant site, than between adjacent sites across the shared edges. On the other hand, Mg-Mg distance across the vacant site is less compressible. It is interesting for understanding of the structure of MgSiO3 ilmenite under high-pressure stable field