High-pressure and high-temperature in situ X-ray diffraction experiments of $(Mg,Fe)SiO_3$ enstatite and ilmenite

K. Fujino*[1](3257), H. Miura[1](3259), T. Shinmei[1](3256), N. Tomioka[1](3255), Y. Hou[1](4009), R. Odawara[1](3995), S. Sato[1](4008), N. Miyajima[2](3254), T. Irifune[3](1224), K. Kuroda[3](3154), and N. Nishiyama[3](3210)

[1] Division of Earth and Planetary Sciences, Hokkaido University, Sapporo 060-0810 Tel: 81-11-706-2728, Fax: 81-11-756-0120, E-mail: fujino@cosmos.sci.hokudai.ac.jp

[2] Institute for Solid State Physics, University of Tokyo, Tokyo 106

[3] Department of Earth Sciences, Ehime University, Matsuyama 790

Introduction

$MgSiO_3$ ilmenite is one of the high pressure polymorphs of enstatite. However, its equation of state (EOS) at high-pressure and high-temperature has not been obtained. These experiments were carried out to obtain the EOS of $MgSiO_3$ ilmenite from in situ X-ray diffraction data at high-pressure and high-temperature.

In situ X-ray diffraction experiments

In situ X-ray diffraction experiments at high-pressure and high-temperature were performed by the SPEED-1500 system at SPring-8. Synthetic $MgSiO_3$ clinoenstatite as a starting material and NaCl as a pressure marker were enclosed in a BN sleeve. The incident synchrotron X-ray beam was directed to the sample through the anvil gap via 50 μm horizontal slit and 300 μm vertical slit.

X-ray intensity measurements were made by the energy dispersive method at fixed 2θ of ~6.0° using white X-ray at pressures up to 21 GPa and temperatures up to 1000 ℃.

Equation of state of $MgSiO_3$ ilmenite

The high temperature EOS for $MgSiO_3$ ilmenite was derived by fitting the obtained pressure-volume-temperature data to the high temperature form of the third order Birch-Murnaghan EOS which is given by the following expression:

$$P = 3/2K_{T,0}[(V_{T,0}/V)^{7/3}-(V_{T,0}/V)^{5/3}]\{1-3/4(4-K_{T,0}')[(V_{T,0}/V)^{2/3}-1]\} \qquad (1)$$

where $K_{T,0}$, $K_{T,0}'$, $V_{T,0}$ are the isothermal bulk modulus, its pressure derivative, and the unit cell volume at temperature T and ambient pressure, respectively. $K_{T,0}$, $K_{T,0}'$ and $V_{T,0}$ were assumed as follows:

$$K_{T,0} = K_{300,0}+(\partial K_{T,0}/\partial T)_P(T-300) \qquad (2)$$

$$K_{T,0}' = K_{300,0}' \qquad (3)$$

$$V_{T,0} = V_{300,0}\exp[\int \alpha_{T,0}dT)] \qquad (4)$$

where $\alpha_{T,0}$ is the thermal expansion coefficient at T and ambient pressure. In this study, we used the following linear expression for $\alpha_{T,0}$:

$$\alpha_{T,0}=a_0+a_1T \qquad (5)$$

Determined parameters are $K_{300,0}'=1.87(5)$, $a_0=2.12\times10^{-5}K^{-1}$, $a_1=1.07(53)\times10^{-8}K^{-2}$ and $(\partial K_{T,0}/\partial T)_P=-0.019(4)GPa/K$ under the constraints of $K_{300,0}=212GPa$ and $\alpha_{300,0}=2.44\times10^{-5}K^{-1}$.