18C/2002G210

Compression behavior of $NiTiO_3$-ilmenite

Takaya NAGAI*, Takehiko TANIMOTO, Masahiro YAMAZAKI
Department of Earth & Space Science, Osaka University,
1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan

Introduction

$NiTiO_3$ has the ilmenite structure with space group *R*-3 at ambient conditions. Ni and Ti atoms are sitting at (0,0,*z*) and O atoms are sitting at a general position (*x*,*y*,*z*). In this structure the O atoms are arranged nearly hcp with the Ni atoms occupying 2/3 of the octahedral sites. It is structurally unique that each Ni octahedron shares a face with an adjacent Ti octahedron in the ilmenite structure. It is important to understand how the ilmenite structure responds to pressure. In this paper, we will report the compression data as the first stage of this investigation. It is noted that our final goal is to understand the compression mechanism from detailed description of the crystal structure as a function of pressure. Especially, pressure response of cation-cation distances across a share face or a share edge seems to be interesting.

Experimental

Reagent-grade of NiO : TiO_2 1 : 1 powders were well mixed and heated at 1500 K for two days. The synthesized powders are confirmed as a single phase of $NiTiO_3$ ilmenite by x-ray powder diffraction.

Sample was pressurized in a diamond anvil cell with a small ruby chip for pressure calibration. Methanol : ethanol 4:1 pressure medium was used.

Angle-dispersive X-ray diffraction measurements were performed at BL18C in the PF using an image plate detector. The monochromatized incident beam to the energy of 20 keV is available and is collimated to 0.04 mm in diameter. Typical exposure time was from 3-4 hours in order to collect well statistical data.

At first, two-dimensional diffraction images were converted to intensity-2θ diffraction patterns using a Program PIP [1]. Then, we carried out a Rietveld analysis using the program RIETAN2000 [2].

Results and discussion

We obtained diffraction data at eight pressure points up to 41.8 GPa. The *a*-axis is slightly compressible rather than the *c*-axis (Fig.1). The pressure-volume data were fit to a second-order Birch-Murnaghan equation of state (Fig.2). The bulk modulus, K_0=240(3) GPa (K'=4) was obtained. This value is much larger than K_0=170 GPa of $FeTiO_3$ ilmenite [3] and surprisingly, larger than K_0=210 GPa of $MgSiO_3$ silicate ilmenite [4]. Liebermann [5] discussed elasticity systematics for the ilmenite structure and the systematics predicts K_0=175 GPa for $NiTiO_3$ ilmenite. However, $NiTiO_3$ ilmenite seems to be an exception of the systematics.

Rietveld structural refinement can provide not only cell parameters but also interatomic distances. Analysis is now progressing and detailed results will come up soon.

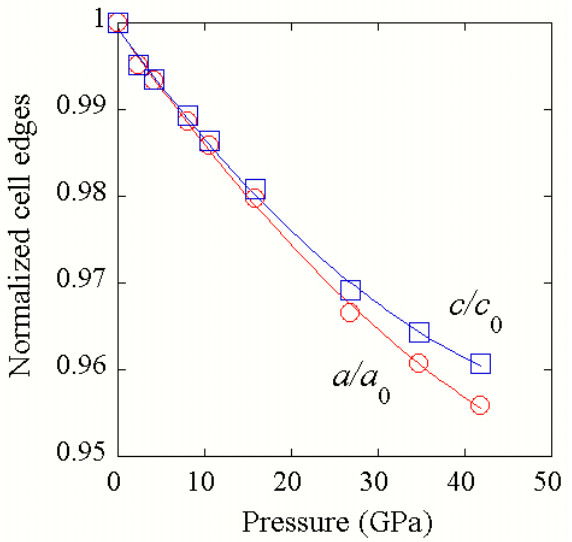

Fig.1 Axial compression data. The solid curves are guides for the eyes

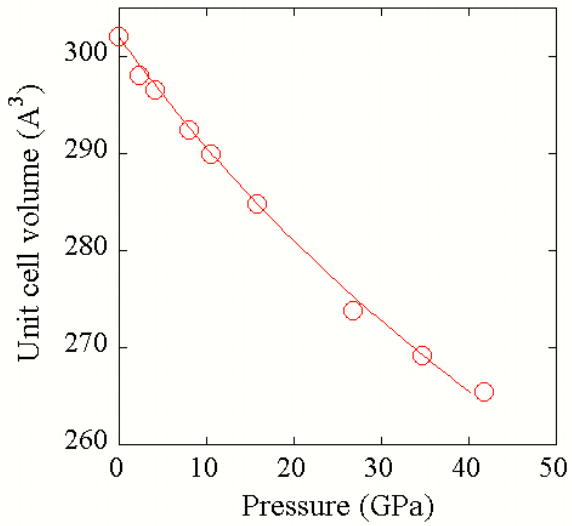

Fig.2 Volume compression data. The solid curve is calculated from the Birch-Murnaghan EOS.

References

[1] Fujihisa & Aoki, Rev.High Press.Sci.Tech.,.8,4 (1998)
[2] Izumi & Ikeda, Mater.Sci.Forum,321,198 (2000)
[3]Wechsler & Prewitt, Am.Mineral.,69,176 (1984)
[4]Weidner & Ito, Phys.Eart Planet.Inter.,40,65 (1985)
[5]Liebermann, Phys.Eart Planet.Inter.,12,P5 (1976)
* nagai@ess.sci.osaka-u.ac.jp