High-pressure behavior of Si-Ge solid solution system

Keiji KUSABA*[1], Takumi KIKEGAWA[2]
[1]IMR, Tohoku Univ., Katahira 2-1-1, Aoba-ku, Sendai 980-8577, Japan
[2]KEK-PF, Tsukuba, Ibaraki 305-0801, Japan

Introduction

There have been many investigations of high-pressure behaviors of silicon and germanium. Compression behaviors of both elements were similar to each other, but decompression behaviors were very different. In the case of Si, the high-pressure phase with the β-tin type structure converted to a body-centered cubic phase (BC8-type phase) in a slow pressure-release process. In the case of Ge, a simple-tetragonal phase (ST12-type phase) was obtained. On the other hand, there are few investigations of Si-Ge solid solution system under high-pressure condition. The aim of this study is to investigate Si-Ge solid solution system in the slow pressure-release process.

Experiment

Six kinds of materials (Ge_xSi_{1-x}; x = 0.00, 0.25, 0.50, 0.75, 0.94 and 1.00) were examined in this study. The powdered material was put in an MgO capsule to protect from chemical reactions. *In-situ* X-ray observation was carried out by the energy-dispersive type X-ray powder diffraction method with MAX80 at AR-NE5C and MAXIII at BL-14C2. The details of the *in-situ* observation method were described in our report [1].

The average decompression rate was about 1GPa/hour in this study.

Result

The BC8-type phase is observed in the chemical composition between x = 0 and x = 0.75 at Ge_xSi_{1-x}, and the ST12-type phase is obtained in the cases of x = 0.94 and 1.00.

Figure 1 shows X-ray diffraction patterns of GeSi as a typical case. The diamond-β-tin type phase transition is observed (Fig. 1-a and –b). In the decompression process, the β-tin type structure reverts to the R8-type structure, which is a rhombohedral-distorted BC8 type structure (Fig. 1-c). The R8-type structure furthermore transforms to the BC8-type structure in the decompression process (Fig. 1-d). At ambient condition, the unit cell parameter of the BC8-type GeSi is a = 6.782(1)Å and the volume of the BC8-type phase is 8.42% smaller that that of the diamond-type phase.

The cubic cell parameter of the BC8-type structure *vs.* atomic ratio is plotted in Fig. 2. The present result is a typical case of "Vegard's rule".

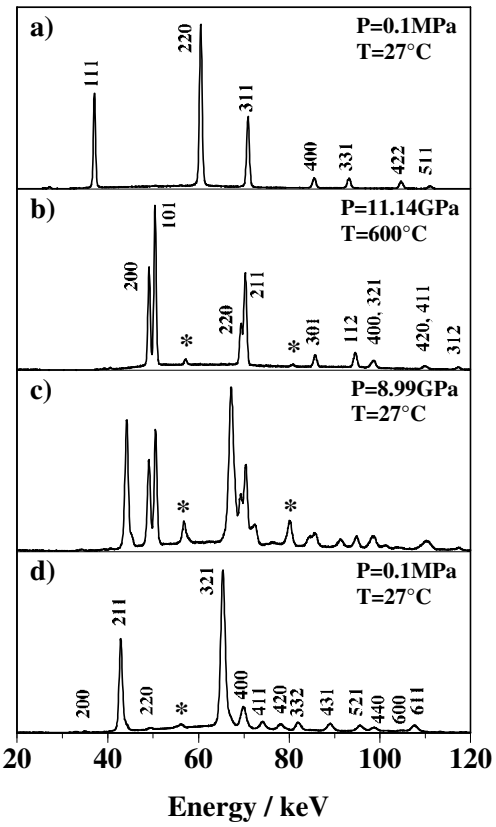

Fig. 1 Powder X-ray diffraction patterns of GeSi, taken at 2θ=600°; a) the diamond-type phase, b) the β-tin type phase, c) a mixture of the β-tin type phase and the R8-type phase and d) the BC8-type phase. Asterisk marks indicate diffraction lines from the MgO capsule.

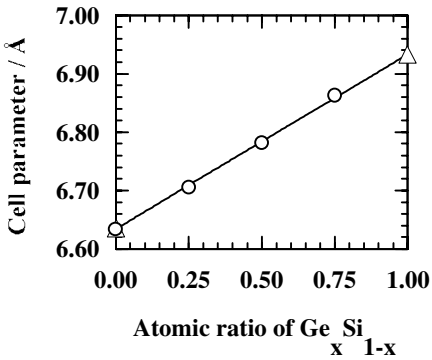

Fig. 2 The cubic cell parameters of the BC8-type phases are plotted as a function of its chemical composition. Circle and triangle marks show the resent results and previous reports, respectively

Reference

[1] Kusaba *et al.*, J. Phys. Chem. Solids 63, 651 (2002).

* kusaba@imr.tohoku.ac.jp