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Pressure-induced phase transition of NdBi with NaCl-type structure

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Introduction

By use of synchrotron radiation, powder X-ray diffraction studied for LnBi (Ln= La, and Pr) with the NaCl-type structure have been carried out up to 30 GPa at room temperature. The structural phase transition of LaBi occurs at about 11.5 GPa. The high-pressure phase of LaBi consists of coexisting of tetragonal (P4/mmm) and cubic (Pm3m) modifications at about 14 GPa.[1] An X-ray study on CeBi and PrBi has been carried out at high pressures. The first-order phase transition in CeBi and PrBi occurs from cubic (Fm3m) to the tetragonal (P4/mmm) and cubic (Pm3m) structures coexist as the high-pressure phase in a wide pressure range.[2,3] The structure of the high-pressure phases of SmBi is a tetragonal (distorted CsCl-type) structure. The structure of the high-pressure phases of LnBi(Ln= Gd and Tm) is a CsCl-type structure.

Using synchrotron radiation we have studied the x-ray diffraction of NdBi with the NaCl-type structure up to 27 GPa at room temperature.

Experimental

NdBi was prepared by reaction of stoichiometric amounts of lanthanum and bismuth in a sealed silica tube at around 850 °C. Using synchrotron radiation the powder x-ray diffraction patterns of NdBi were measured with a diamond-anvil cell and the imaging plate up to 27 GPa at room temperature. Incident beam was monochromatized by Si(111) double crystal to a wavelength of 0.62 Å. The pressure in the diamond-anvil cell was determined from a pressure shift in the sharp R-line fluorescence spectrum of ruby. A fluorinert solution was used as the pressure transmitting fluid.

Results and Discussion

Figure 1 shows powder x-ray diffraction patterns of NdBi at high pressures. The profile indicates characteristic lines of the NaCl-type structure and Bi impurity lines at around 1 atm. The first-order phase transition in bismuth impurity occurs from rhombohedral to cubic structure at about 10 GPa. The d-values of 111, 200, 220, 222, 400 and 420 lines of NdBi decrease with increasing pressure up to 15 GPa. New diffraction lines appear above 16.8 GPa and grow with increasing pressure. The reflections of the NaCl-type structure disappear around 21.1 GPa. The 110 line of the CsCl-type structure expected as the high-pressure form is split into two lines 110 and 101 in the tetragonal (distorted CsCl-type) structure. Crystal data of the single phase at 21.1 GPa are a = 3.850(4) Å, c = 3.28 (1) Å, c/a = 0.85 and V = 48.6(2) Å^3. The high-pressure phase of NdBi is isostructural with that of SmBi and NdX (X= P, As and Sb).

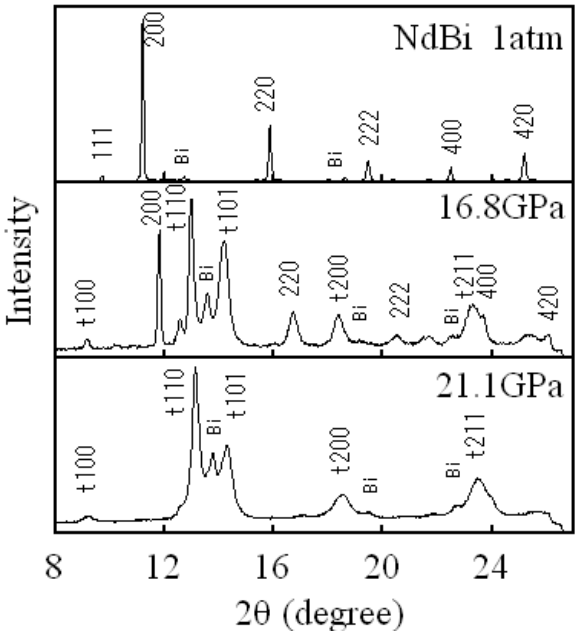

Fig. 1. Powder x-ray diffraction pattern of NdBi at high pressures.

References

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