Phase transition of SmAs with NaCl-type structure at high pressures

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Introduction

Using synchrotron radiation, x-ray diffraction of LnP(Ln = La, Ce, Pr, Nd, Sm, Gd, Tb, Tm and Yb) has been studied up to 61 GPa at room temperature. First-order phase transitions of LnP with the crystallographic change occur at high pressures. The structure of the high pressure phases of LnP(Ln = La, Pr and Nd) is a body center tetragonal (BCT) structure which can be seen as the distorted CsCl-type structure.[1] The compression curves of CeAs have been investigated up to 32 GPa. The phase transition in this arsenide occurs at around 17 GPa; the structure changes from the NaCl-type to the CsCl-type structure.[2] However, the high pressure structural behavior of other lantanide monoarsenides with the NaCl-type structure has not been studied.

Using synchrotron radiation we have studied the x-ray diffraction of SmAs with the NaCl-type structure up to 45 GPa at room temperature. The pressure-induced phase transition for the arsenide is observed above 34 GPa.

Experimental

SmAs was prepared by reaction of stoichiometric amounts of each rare earth metal and arsenic in a sealed silica tube at around 900 °C. The compounds prepared by us were characterized by powder x-ray diffraction using Cukα radiation and silicon as a standard.

Using synchrotron radiation the powder x-ray diffraction patterns of SmAs were measured with a diamond-anvil cell and a imaging plate up to 45 GPa at room temperature. Incident beam was monochromatized by Si(111) double crystal to a wavelength of 0.4959 Å. The pressure in the diamond-cell was determined from a pressure shift in the sharp R-line fluorescence spectrum of ruby. A 4:1 methanol-ethanol solution was used as the hydrostatic pressure fluid.

Results and Discussion

Figure 1 shows powder x-ray diffraction patterns of SmAs at high pressures. The profile indicates only characteristic lines of the NaCl-type structure at around 1.9 GPa. The d-values of 111, 200, 220, 311, 222, 400, 331, 420, 422, 511, 600, 620 and 533 lines of SmAs decrease with increasing pressure up to 33 GPa. New diffraction lines appear above 34 GPa and grow with increasing pressure. Low and high pressure phases coexist in the wide pressure range. A single phase of the new high pressure phase is obtained above 46 GPa. When the pressure is removed, the diffraction lines of the NaCl-type structure reappear at around 15 GPa. The x-ray diffraction pattern of the high pressure phase of SmAs cannot be assigned by the index of the CsCl-type and the BCT structures. The structure of SmAs is not determined at high pressure.

References

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2) A. Werner, H.D. Hochheimer, R.L. Meng and Bucher, Phys. Lett., A97, 207(1983).

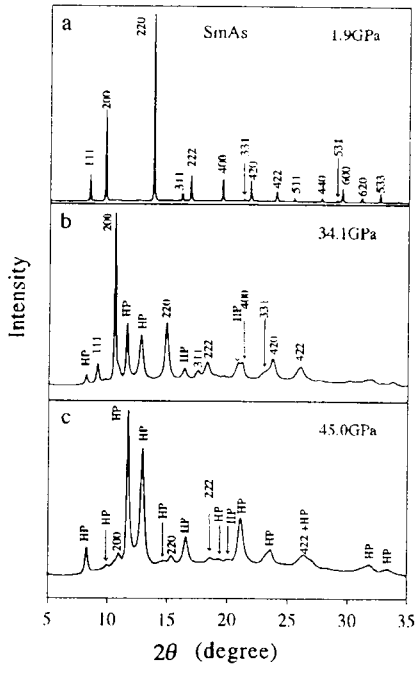

Fig.1 Xray diffraction patterns of SmAs at various pressures at room temperature. HP means the high pressure phase.