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X-RAY DIFFRACTION STADY OF SKUTTERUDITE COMPOUNDS AT HIGH PRESSURES

Ichimin SHIROTANI [1], Takashi NORO [1], Junichi HAYASHI [1], Chihiro SEKINE[1], Ram GIRI[1] and Takumi KIKEGAWA[2]

[1]Muroran Institute of Technology, 27-1, Mizumoto, Muroran-shi 050-8585, Japan

[2]KEK-IMSS, Tsukuba, Ibaraki 305-0801, Japan

Introduction

Ternary metal pnictides with a general formula LnT_4X_{12} (Ln = lanthanide; T = transition metal; X = pnicogen) crystallize with a filled skutterudite-type structure. This structure is cubic, space group Im-3, Z = 2. The skutterudite compounds show interesting electrical and magnetic properties at low temperatures. Using synchrotron radiation, we have studied the powder x-ray diffraction for P- and Sb-based binary and filled skutterudites at high pressures, and obtained the bulk modulus of these skutterudites

Experimental

P- and Sb-based skutterudite compounds were prepared by reaction of each metal and red phosphorus or antimony powders at high pressure and high temperature [1]. Using synchrotron radiation, powder x-ray diffraction patterns of these compounds were measured with a diamond-anvil cell and an imaging plate at high pressures [2]. The pressure in the diamond-anvil cell was determined from a pressure shift in the sharp R-line fluorescence spectrum of ruby grain. A 4:1 methanol-ethanol solution was used as pressure medium.

Results and discussion

Figure 1 shows the relative cell volume (V / V_0) vs. pressure curves for $CeOs_4P_{12}$ and $CeOs_4Sb_{12}$. The cell volume with the skutterudite-type structure monotonically decreases with increasing pressure up to 10 GPa. The pressure vs. volume curve for both compounds is fitted by a Birch equation of state. Bulk moduli of $CeOs_4P_{12}$ and $CeOs_4Sb_{12}$ are 150 ± 5 GPa and 85 ± 5 GPa, respectively. The bulk modulus of the phosphide is about two times that of the antimonide. Figure 2 shows the ratio of the lattice constant (a / a_0) for $CeFe_4P_{12}$ and $CeFe_4Sb_{12}$ at high pressures. The lattice constants of both compounds monotonically decrease with increasing pressure up to about 10 GPa. The antimonide is sensitive to pressure compared with the phosphide. The pressure vs. volume curve for both compounds is fitted by a Birch equation of state. Bulk moduli of both skutterudites are 162 ± 4 GPa for $CeFe_4P_{12}$ and 88 ± 4 GPa for $CeFe_4Sb_{12}$. The bulk modulus of $CeFe_4P_{12}$ is about two times that of $CeFe_4Sb_{12}$.

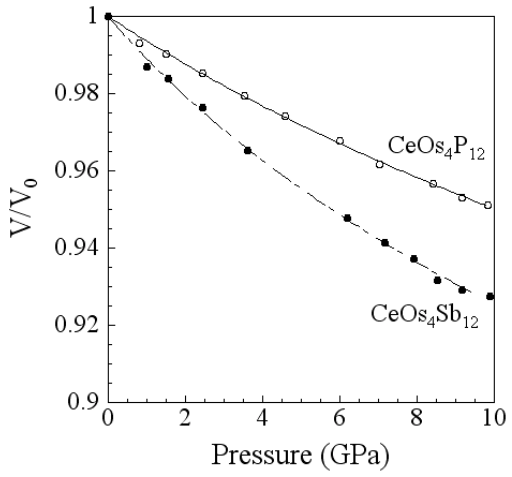

Fig. 1 The relative cell volume (V / V_0) vs. pressure curves for $CeOs_4P_{12}$ and $CeOs_4Sb_{12}$.

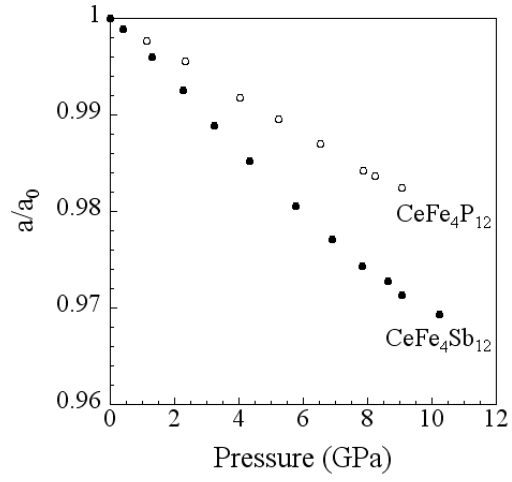

Fig. 2 The ratio of the lattice constant (a/a_0) for $CeFe_4P_{12}$ and $CeFe_4Sb_{12}$ at high pressures.

References

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* sirotani@eee.elec.muroran-it.ac.jp