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X-ray diffraction study of filled skutterudite $BaRu_4As_{12}$ at high pressures

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Introduction

Ternary metal arsenides with a general formula RT_4As_{12} (R= rare earth; T= transition metal) crystallize with a filled skutterudite-type structure. $LaRu_4As_{12}$ show the superconducting transition at 10.3 K [1]. We have prepared a new filled skutterudite $BaRu_4As_{12}$ at high temperatures and high pressures. The electrical property of $BaRu_4As_{12}$ has been studied at low temperature. This arsenide shows the metallic behavior down to 2 K. The crystal structure of $BaRu_4As_{12}$ was refined by the Rietveld analysis of the x-ray powder diffraction data at ambient pressure [2].

Using synchrotron radiation, we have studied the powder x-ray diffraction for filled skutterudite $BaRu_4As_{12}$ up to 10 GPa at room temperature. A bulk modulus was estimated from the volume vs. pressure curve fitted by a Birch equation of state.

Experimental

Using a wedge-type cubic-anvil high-pressure apparatus, $BaRu_4As_{12}$ was prepared at high temperatures and high pressures. The powder x-ray diffraction patterns of $BaRu_4As_{12}$ were measured with a diamond-anvil cell (DAC) and the imaging plate up to 10 GPa at room temperature. The high-pressure diffraction experiments with synchrotron radiation were performed at the beam line BL-18C. Incident beam was monochromatized by Si(111) double crystal to a wavelength of 0.6199 Å. The x-ray beam was collimated to 100 μm in diameter. Pressure in the DAC was determined from a pressure shift in the sharp R-line fluorescence spectrum of ruby. 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 for $BaRu_4As_{12}$ and $LaRu_4As_{12}$. The cell volume with the skutterudite-type structure monotonically decreases with increasing pressure up to 10 GPa. The compression curve for both skutterudites is fitted by a Birch equation of state. Bulk moduli (B_0) of $BaRu_4As_{12}$ and $LaRu_4As_{12}$ are 127.0 ± 0.2 GPa and 136 ± 3 GPa, respectively. The B_0 value of $BaRu_4As_{12}$ is smaller than that of $LaRu_4As_{12}$. Lattice constant, ionic radius of barium metal and lanthanum metal and bulk modulus of $BaRu_4As_{12}$ and $LaRu_4As_{12}$ are summarized in table1. The bulk modulus increases with decreasing lattice constant. It has been understood that the bulk modulus decreases when the lattice constant expands with the atom of a large ionic radius.

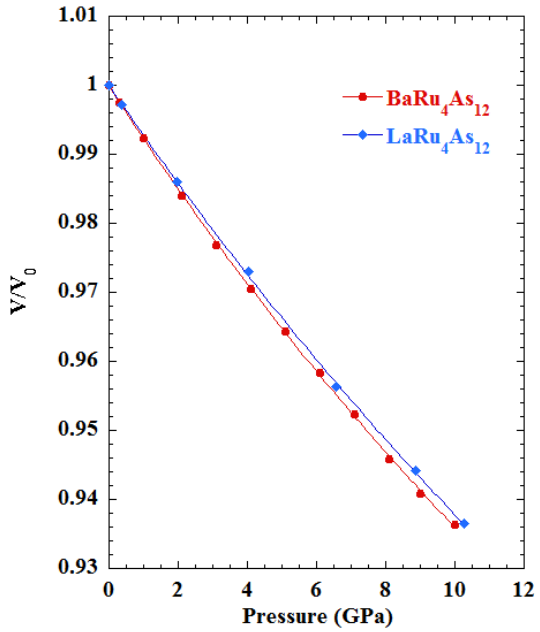

Figure 1 Relative cell volume plotted as a function of pressure for $BaRu_4As_{12}$ and $LaRu_4As_{12}$.

Table 1 Lattice constant, ion radius of barium metal and lanthanum metal, bulk moduls of $BaRu_4As_{12}$ and $LaRu_4As_{12}$.

	$BaRu_4As_{12}$	$LaRu_4As_{12}$
Lattice constant (Å)	8.5555	8.5081
Ionic radius (Å) of Ba^{2+} and La^{3+}	1.42	1.16
B_0 (GPa)	127.0 ± 0.2	136 ± 3

References

[1] I. Shirotani et al., Phys. Rev. B 56 7866 (1997).
[2] K. Takeda et al., J. Phys. : Conf. Ser., 215 012130 (2010).

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