

X-ray diffraction study of filled skutterudite superconductors at high pressures

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Ichimin SHIROTANI¹, Takumi KIKEGAWA²¹ Muroran Institute of Technology, Muroran, Hokkaido 050-8585, Japan² KEK-IMSS, Tsukuba, Ibaraki 305-0801, Japan**Introduction**

Ternary metal pnictides with a general formula RT_4X_{12} (R = lanthanide; T = transition metal; X = pnictogen) crystallize with a filled skutterudite-type structure. This structure is cubic, space group Im-3, $Z = 2$. The filled skutterudite compounds LaT_4P_{12} ($T = Fe, Ru$ and Os) are superconductors with the superconducting transition temperatures (T_c 's) = 4.1, 7.2 and 1.8 K [1, 2]. The bulk modulus is also obtained from the volume vs. pressure curve fitted by a Birch equation of state [3].

We have prepared a new filled skutterudite YT_4P_{12} ($T = Fe$ and Os) at high temperatures and high pressures, and have found the superconducting transition at around 7 K for YFe_4P_{12} and 1.8K for YOs_4P_{12} [4, 5]. Using synchrotron radiation, we have studied the powder x-ray diffraction for filled skutterudites YT_4P_{12} ($T = Fe$ and Os) at room temperature and high pressures, and obtained the bulk modulus of these skutterudites.

Experimental

Using a wedge-type cubic-anvil high-pressure apparatus, YT_4P_{12} ($T = Fe$ and Os) were prepared at high temperatures and high pressures. The powder x-ray diffraction patterns of YT_4P_{12} ($T = Fe$ and Os) were measured with a diamond-anvil cell (DAC) and the imaging plate up to 10 GPa at room temperature. Incident beam was monochromatized by Si(111) double crystal to a wavelength of 0.6199 Å. The x-ray beam was collimated to 60 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 YT_4P_{12} ($T = Fe$ and Os). 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 of YFe_4P_{12} and YOs_4P_{12} are 144 ± 2 GPa and 189 ± 4 GPa, respectively. Table 1 shows lattice constant at ambient pressure, T_c and bulk modulus for LaT_4P_{12} ($T = Fe, Ru$ and Os) and YT_4P_{12} ($T = Fe$ and Os). The results show that the bulk modulus simply dependent on the lattice constant. The bulk modulus of these skutterudites increases with increasing lattice constant.

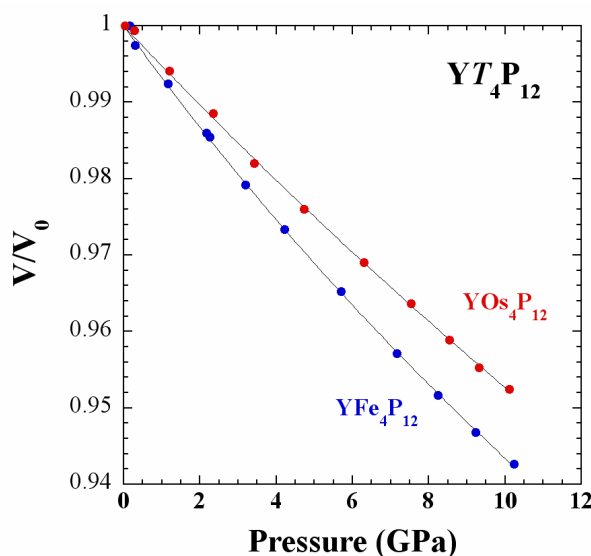


Fig. 1 The relative cell volume (V/V_0) vs. pressure curves for YFe_4P_{12} and YOs_4P_{12} .

Table 1 Lattice constant, T_c and bulk modulus for LaT_4P_{12} ($T = Fe, Ru$ and Os) and YT_4P_{12} ($T = Fe$ and Os).

Compound	Lattice constant (Å)	T_c (K)	Bulk modulus (GPa)
YFe_4P_{12}	7.789	7	144
YOs_4P_{12}	8.0615	3	189
$LaFe_4P_{12}$ *	7.8316	4.1	150
$LaRu_4P_{12}$ *	8.0605	7.2	172
$LaOs_4P_{12}$ *	8.0844	1.8	190

* : Ref. [3]

References

- [1] G.P. Meisner, Physica 108B (1981) 763.
- [2] L.E. DeLong *et al.*, Solid State Commun., 53 (1985) 119.
- [3] I. Shirotnani *et al.*, J. Phys.: Condens. Matter 16 (2004) 7853.
- [4] I. Shirotnani *et al.*, J. Phys.: Condens. Matter 15 (2003) S2201.
- [5] K. Kihou *et al.*, Mater. Res. Bull., 39 (2004) 317.

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