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X-ray study of new filled skutterudite compounds at high pressure

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Ternary metal pnictides with a general formula RT_4X_{12} (R= lanthanide, T= transition metal, X= pnicogen) crystallize with a filled skutterudite-type structure. This structure is cubic, space group $Im\bar{3}$ and Z= 2. We have prepared a new filled skutterudite RT_4P_{12} (R= Gd, Dy and Y, T= Fe, Ru and Os) at high temperature and high pressures. Using synchrotron radiation, the crystal structures of new filled skutterudites were refined with Rietveld methods at ambient pressure [1]. The powder x-ray diffraction of new skutterudites has systematically measured with a diamond-anvil cell and an imaging plate at room temperature and high pressure (up to 10 GPa). The bulk modulus is obtained from the volume vs. pressure curve fitted by Birch equation of state [2]. Figure 1 shows the relative cell volume (V/V_0) vs. pressure curve for $DyRu_4P_{12}$. The cell volume with the skutterudite-type structure monotonically decreases with increasing pressure up to 10.3 GPa. The compression curve for $DyRu_4P_{12}$ is fitted by a Birch equation of state. Bulk modulus of $DyRu_4P_{12}$ is 190 ± 2 GPa. This result is good agreement of other ruthenium phosphide. The bulk modulus simply dependent on the lattice constant. The value of phosphides is about two times larger than that of antimonides.

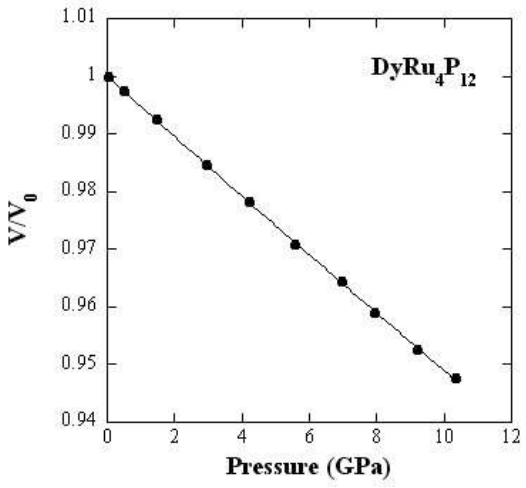

Figure 1: The relative cell volume (V/V_0) vs. pressure curve for $DyRu_4P_{12}$.

References

[1] I. Shirotani et al., Z. Naturforsch. 61b (2006) 1471-1476.
[2] I. Shirotani et al., J. Phys.: Condens. Matter, 16 (2004) 7853.