【S-16】

# Magnetic structures of CrPt3 by first-principles calculation

Youngsoo Kwon, T. H. Rho, Sangsoo Lee, and Soon C. Hong
Department of Physics, University of Ulsan, Ulsan 690-749

The ordered alloys $Cu_3Au(Ll_2)$ type crystal structures have been attracting much interest because they reveal a rich variety of magnetic ordering. $VPt_3$ and $CrPt_3$ are ferrimagnetic in sense that the moment of Pt atoms are antiparallel to that of the transition metal atom, $MnPt_3$ and CoPt3 are ferromagnetic, and FePt3 is antiferromagnetic.

The calculations were performed using the full-potential linearized augmented plane wave method (FLAPW) with general gradient approximation (GGA) for exchange-correlation potential.

To investigate the magnetic structures we assumed four possible magnet structures, a ferromagnetic structure and three different antiferromagnetic structures: (i) type-1 antiferromagnetic coupling along the Cr[100] direction; (ii) type-2 antiferromagnetic coupling along the Cr[110] direction; (iii) type-3 anti-ferromagnetic coupling along the Cr[111] direction.

The ferromagnetic structure was found to be most stable from the calculations of total energy with the lattice constant. Type-3 was calculated to be next most stable. In the reference of ferromagnetic state their energy differences are 139, 157, and 60 meV/Cr-atom for type-1, 2, and 3, respectively. The calculated lattice constants for the four different magnetic structures were slightly larger, 1.12, 1.22, 1.23, and 1.26 % than that of experiment (3.88Å) for ferromagnet and antiferromagnet type-1, 2, and 3, respectively. The magnetic moments of the Cr ferromagnetic state was calculated as 2.78 $\mu$B. The Cr is coupled antiferromagnetically to that of Pt(-0.05 $\mu$B). This is good agreement with an experiment1. The magnetic moments in the antiferromagnetic states are calculated to be 2.81, 2.81, and 2.88 $\mu$B for type-1, 2, and 3, respectively.

1. V. N. Andonov. Phys. Rew. B. 64 (2001) 024402-1