A-07

Magnetic and electronic structures of Mn_2As by first principles calculations

Gul Rahman, Sunglae Cho, and Soon Cheol Hong@

Department of Physics, University of Ulsan

Early in the 1960s, it was shown by experiments[1,2] that Mn_2As was a layered AFM metal with a tetragonal Cu_2Sb crystal structure. Magnetic-susceptibility and specific heat measurements by Yuzuri and Yamada[1] indicated that Mn_2As had a Neel temperature of 573 K. Based on experimental results and molecular field theory analysis, it was concluded that the antiferromagnetic ordering was stable in general, and predicted that an antiferromagnetic-ferrimagnetic transition might occur at low temperature. The magnetic moments given by neutron-diffraction studies[2] on the powder specimens of Mn_2As were 3.7 and 3.5 Bohr magnetrons (μ_B) for the two kinds of Mn atoms, Mn (I) and Mn (II) respectively. The magnetic moments are perpendicular to the c axis of the tetragonal structure. The electronic and magnetic properties of Mn_2As were studied by Zongxian Yang et al[3] by using self consistent tight binding linear muffin-tin orbital (TB-LMTO) method. They found that the ground state of Mn_2As is in the layered antiferromagnetic metal phase.

Mn_2As has a tetragonal Cu_2Sb crystal structure[1,2] as shown in fig. 1, which is the magnetic unit cell with the *c* axis being twice that of the unit cell used in crystallography (the upper half of the unit cell shown in Fig. 1), In the crystal lattice of Mn_2As there are two kinds of cation sites Mn (I) and Mn (II) which are surrounded tetrahedrally and octahedrally respectively, by arsenic atoms. The Mn (I) atoms are at positions ~0, 0, 0 and 0.5, 0.5, 0. The Mn (II) and As atoms are at positions 0, 0.5, *z* and 0.5, 0, -*z*. The values of the parameter *z* are 0.330 and 0.265 for Mn (II) and As atoms respectively, which are the same values used for Fe (II) and As in Fe_2As. Mn_2As is very interesting material with many peculiar features. Its presence at the interface or in the spacer layer of trilayer system might affect the magnetic properties of the systems.

We employed spin polarized, full potential linearised augmented plane wave (FLAPW) method in generalized gradient approximation (GGA) adopted for the exchange-correlation functional. We used the crystallographic unit cell shown in the upper part of with a=3.78 Å and c=6.28 Å for our calculations. For this unit cell we considered

three types of spin ordering i.e. Ferromagnetic (FM), Ferrimagnetic (FIM) and antiferromagnetic (AFM). The calculated total energy and density of state for this system in different spin configurations shows that antiferromagnetic metal is the ground state. The magnetic moments are 2.32 μ_B and 3.44 μ_B per Mn atom for Mn (I)and Mn (II) respectively.

Our calculated magnetic moment of Mn (II) is very close to the experimental[2] and theoretical[3] value whereas for Mn (I) there is a disagreement between experiment and theoretical calculations. Yuzuri and Yamada[1] found the experimental magnetic moment for Mn(I) is 3.7 μ_B while Zongxian Yang et al[3] showed 1.87 μ_B using (TB-LMTO) method while our precise ab-initio FLAPW calculations shows the magnetic moment 2.32 μ_B for Mn (I)

In this meeting we will also present the magnetic and electronic structure of Mn_2As for the magnetic unit cell shown in fig.1 in different spin ordering i.e FM, FIM, AFM1 and AFM2.

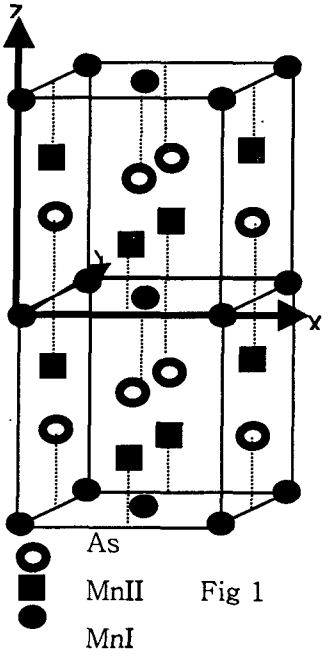

Fig 1

*Supported by the Basic Research Program (R01-2004-000-10957-0) of KOSEF and via eSSC at POSTECH

References

[1] M. Yuzuri and M. Yamada, J. Phys. Soc. Jpn. **15**, 1845 (1960)

[2] E. Austin, E. Adelson, and W. H. Cloud, J. Appl. Phys. **33**, 1356 (1962)

[3] Zongxian yang, kaiming zhang, and xide xie Phys. Rev. B **58** 339(1998)