AT23

Magnetic Properties of Carbon Doped ZnO: First Principle Calculation

Dongyoo Kim and Jisang Hong*

Departments of Physics, Pukyong National University, Busan 608-737, Korea

*Corresponding author: Jisang Hong, e-mail: hongJ@pknu.ac.kr

Recently, experimental and theoretical study reported that Carbon doped ZnO has ferromagnetism at room temperature [1]. Through the full potential linearized augmented plane wave method, we have explored the magnetism of 8.3% Carbon doped wurtize ZnO varying the relative position between two C atoms. The 2 x 2 x 3 unit cell size is considered in our calculations. This corresponds to the lattice parameters 6.499 Å, 6.499 Å, and 15.6163 Å in the a-, b-, and c-directions, respectively. This means that we have 48 atoms in a unit cell. We have found that the magnetic moment of C depends on relative position of C. When atomic distance between two C atoms is 6.136 Å (Type I), the magnetic moments of two C atoms are 0.44 μ_B and 0.43 μ_B, respectively. However, two C atoms have magnetic moment of 0.22 μ_B with atomic distance 3.249 Å (Type II). In addition, we have compared the total energy between Type I and Type II, and Type II is more stable. This may imply that the C atoms tend to get closer, not preferring uniform distribution. Also, we will present the X-ray magnetic circular dichroism (XMCD) spectra.

This work was supported by the Korea Research Foundation Grant funded by the Korean Government (MOEHRD) (KRF-2006-331-C00105)

REFERENCES

[1] H. Pan, J.B. Yi, L. Shen, R. Q. Wu, J. H. Yang, J. Y. Lin, Y.P. Feng, J. Ding, L.H. Van and J. H. Yin, Phy. Rev. Let. 99, 127201 (2007).

AT24

Magnetism of Mn δ-doped GaSb Digital Alloy: Density Functional Study

Oryong Kwon, Won Seok Yun, and Soon Cheol Hong*

Department of Physics, University of Ulsan, Ulsan 680-749, Republic of Korea

* Corresponding author: e-mail schong@mail.ulsan.ac.kr, Phone: +82 52 259 2331, Fax: +82 52 259 1693

As new systems with high Curie temperature and large magnetic moments, digital alloy systems of transition metal δ-doped semiconductors have been suggested [1-2]. In this study, we investigated magnetism of Mn δ-doped GaSb where the atoms were allowed fully relaxed by calculation of total energy and force, using the all-electron full-potential linearized augmented plane wave method. General gradient approximation was employed to describe the exchange-correlation interaction among electrons. We consider two different systems to take the effect of an imperfect interface on the magnetism into account; clean δ-doped and replaced the nearest neighbor Ga with Mn. We have obtained quite interesting results. As well as the replaced system is more stable than the clean δ-doped system, the total energy difference (180 meV) between the AFM and the FM states is also larger in the replaced system compared to that (90 meV) of the clean one, which may result in higher Curie temperature of the replaced system [3].

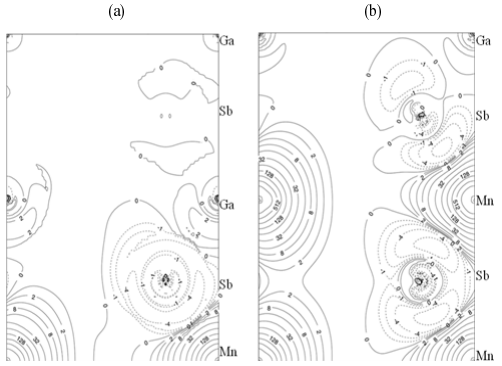

Fig. 1. Spin density contours on the (014) plan of each system in (a) clean δ-doped (b) defected systems in FM state. The solid (dashed) lines represent positive (negative) polarization.

This work was supported by by KOSEF through NRL program (Grant 2006-02202).

REFERENCES

[1] E. Johnson-Halperin et al., Phys. Rev. B **68**, 165328 (2003).
[2] X. Chen et al., Appl. Phys. Lett. **81**, 511 (2002).
[3] V. Y. Irkhin et al., Phys. Rev. B **60**, 1082 (1999).