The magnetic properties of digital magnetic heterostructures δ-doped with Cr or Mn

Lee-Hyun Cho*, B. Bialek, and Jae Il Lee
Department of Physics, Inha University, Incheon 402-751, Korea

1.Introduction

Due to the possibility of application forspintronics, diluted magnetic semiconductors (DMSs), composed of a semiconductor and a metal, have been widely investigated [1,2]. Recently, the magnetic properties of GaAs-based digital magnetic heterostructures (DMHs), d-doped with Cr or Mn, have been reported [1]. The obtained results were ambiguous: the half-metallicity of the compounds was revealed when the calculations were carried out with local spin density approximation, but when many-body correlations were additionally concerned, the half-metalic gaps in the electronic structure of the compounds were closed.

In order to investigate in detail the nature of possible half-metallicity in GaAs/MeAs (Me=Cr, Mn) DMHs, we studied the electronic and magnetic properties of several superstructures, in which the thickness of the GaAs spacer varied from 5 to 7 layers.

2. omputational model and method

Each superstructure consisted of 8 repeated layers in [001] direction. The least doped structure was the one with 7 layers of GaAs sandwiched with a layer of GaAs, in which 50% of Ga atoms in one layer were substituted by the transition metal atom (Cr or Mn). The system richest in dopants consisted of 5 layers of GaAs sandwiched with 3 layers of MeAs (Me=Cr, Mn). For example, in Fig. 1 we show a schematic layer-by-layer atomic structure of $(Ga\text{-}MnAs)_1/(GaAs)_7$supercell.

All the calculations were performed with the use of an all-electron full-potential linearized augmented plane wave (FLAPW) method within the generalized gradient approximation [3-5]. The Kohn-Sham equation was solved self-consistently. Lattice harmonicswith $l \leq 8$ were employed to expand the charge density, the potential, and the wavefunctions inside muffin-tin radii of 2.20 bohr for transition metals and 2.30 bohr for post-transition metals. Allcore electrons were treated fully relativistically, while valence states were treated scalarrelativistically.

3. Results

Among the ten investigated systems, we found an integer value of the total magnetic moment (MM) per formula unit in eight of them. The two systems for which the calcun atoms, i.e. $(MnAs)_3/(GaAs)_5$ and $(Ga\text{-}MnAs)_1/(MnAs)_1/(Ga\text{-}Mn,As)_1/(GaAs)_5$. Interestingly, the systemsof tlated total MMs per formula units were non-integer were those with the largest amount of doped Mhe same composition in which Mn is substituted by Cr atom exhibit half-metallicity. The results obtained in ourcalculations let usanalyze charge density distribution within the investigated systems and, specifically, the changes in the electronic density due to the various amount of Mn or Cr dopants. The presence of magnetic centers in the superstructures rather weakly influences the properties of the Ga atoms in the structures. The atoms do not gain a significant magnetic moment due to the interactions with Mn or Cr. As for As atoms, if the structures contain two or more transition metal atoms per

supercell, the As atom closest to the magnetic center gains negative MM that may be as large as–0.254 μ_B in the $(CrAs)_2/(GaAs)_6$.

In our paper, we will present a detailed discussion of the quantitative results and we will analyze the derived density of electronic states for the investigated systems.

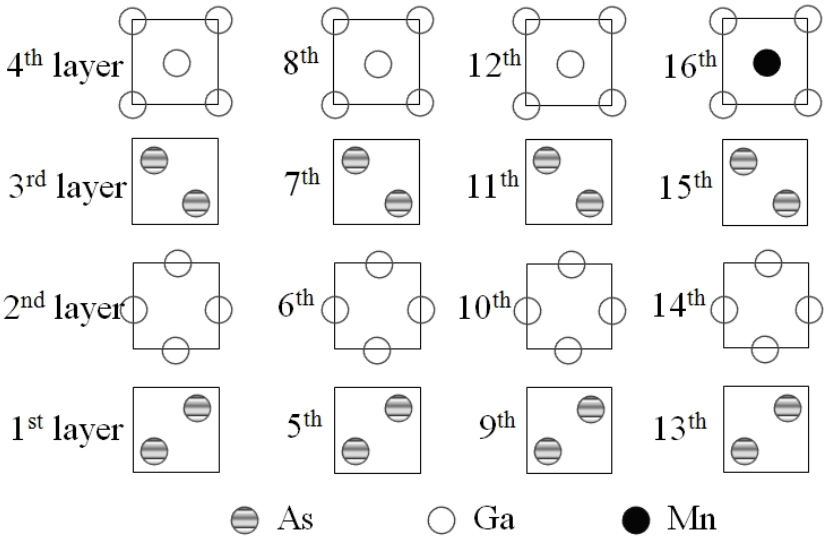

Fig. 1. A schematic view of the subsequent atomic layers in $(Ga\text{-}MnAs)_1/(GaAs)_7$supercell.

References

[1] F. Beiuseanu, C. Horea, E. –V. Macocian, T. Jurcut, L. Vitos, and L. Chioncel, Phys. Rev. B 83, 125107 (2011).

[2] Y. H. Chang and C. H. Park, Phys. Rev. B 76, 125211 (2007).

[3] E. Wimmer, H. Krakauer, M. Weinert, and A. J. Freeman, Phys. Rev. B 24, 864 (1981).

[4] M. Weinert, E. Wimmer, and A. J. Freeman, Phys. Rev. B 26, 4571 (1982).

[5] J. P. Perdew and Y. Wang, Phys. Rev. B 45, 13244 (1992).

[6] W. Kohn and L. J. Sham, Phys. Rev. A 140, 1133 (1965).

[7] D. D. Koelling and B. N. Harmon, J. Phys. C 10 3107 (1977).