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First principle calculations of zinc blende superlattice surfaces and multilayers with ferromagnetic dopants

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In order to understand conditions for appearance of half-metallicity in MnAs/AsGa(001) digital alloy superlattices, we calculated the electronic and magnetic structure of zinc blende multilayers in various ab initio supercell geometries for ferromagnetic dopants (Fe, Cr). The bulk atomic structure model is extended allowing consideration of the surface ferromagnetic metal monolayer (Fe, Cr) in the slab approximation. The calculations were performed using the density functional theory (DFT) method within the full-potential and linearized augmented plane-wave (LAPW) approach. This work presents detailed information about total and atom projected density of states (DOS) functions in the surface region of the investigated systems. Our interest was to look for common trends and differences in the electronic structures for different locations of ferromagnetic adatoms and surface monolayer (Fe, Cr) in the zinc blende digital alloy surfaces and multilayers.

Key words: *digital ferromagnetic heterostructure; density functional theory; half-metal*

1. Introduction

Use of the molecular beam epitaxy (MBE) for microfabrication of magnetic semiconductor heterostructures allowed fabricating magnetic semiconductor multilayer structures, i.e., producing controlled magnetism via changes in the number of magnetic layers and the direction of spin momentum.

Investigating and synthesizing new spintronic materials has a great practical importance due to their application in future information technology and electronic devices. Among all proposed materials, semiconductors made by doping with magnetic ions (V, Cr, Mn, Fe, Co, and Ni) or preparing a hybrid structure of magnetic element with a semiconductor [1] exhibit the most promising properties. The (Ga,Mn)As heterostructures have opened a completely new method to combine magnetism with charge transport in well known semiconductor device structures.

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Half-metallic (HM) random (diluted) and digital ferromagnetic dopants attract much interest as they have only one occupied set of spin density of states at the Fermi level, and thus should in principle be capable of 100% polarized spin current injection. They have been examined as the source of spin polarized electrons for innovative spintronic devices and sophisticated experiments [2]. Digital ferromagnetic heterostructures (i.e., digital alloys) have been fabricated by alternately depositing semiconductors such as GaAs and one submonolayer MnAs using low temperature molecular beam epitaxy, because only 0.5 ML of Mn can be deposited with this technique.

Theoretical calculations focused on conventional alloys containing randomly distributed Mn in the semiconductor host, predict T_C on the basis of Zenner mode [3] and prove that an increase of the Mn concentration increases the Curie temperature of the random alloy $Ga_{1-x}Mn_xAs$ systems. The highest critical temperatures observed so far in (Ga,Mn)As have been in the range 50–110 K but the theory predicts that even at room temperature magnetism could be achievable. One approach to increasing T_C is to replace random heterostructures with digital ferromagnetic heterostructures (DFH). The density functional theory (DFT) calculations for zinc blende (ZB) superlatices and their surfaces have been performed by few authors [4–6]. It has been reported that the half-metallicity of MnAs/AsGa digital alloys can be destroyed by Fe monolayers (0.5 ML) embedded in these zinc blende superlattice materials [7].

2. Method of calculation and results

The half-metallic properties of a M/MnAs/GaAs(001) (M = Fe, Cr) digital alloy superlattice surfaces have been investigated within the density functional theory, using the highly precise all-electron full-potential linearized augmented plane-wave (FP LAPW) method within the generalized gradient approximation (GGA Perdew –Burke–Ernzerhof 96) for the exchange and correlation functionals, implemented in WIEN2k program package [8].

Surfaces have been modelled using a supercell-slab model with periodic boundary conditions containing a set of 12 or 15 atoms (Fig. 1). Calculations have been performed for zinc blende (ZB) tetragonal unit cell geometry with $a_0/\sqrt{2}$ in the **a** and **b** directions for different spin channels with optimized lattice constant. Different spin channels self consistent slab calculations have been performed for a **k**-point set equivalent to one **k** point, until obtaining convergence and to four **k** points for DOS convergent calculations. All DOS surface (multilayer) calculations were performed after the surface relaxation calculations.

Each DFH slab (Fig. 1) was constructed by considering three GaAs tetragonal unit cells (four atoms in the cell), surface metallic 1 ML and a vacuum of 8–10 MLs, aligned along the *x* direction. Further details of the method have been published in Ref. [1]. One Ga atomic monocrystal plane in the first and third AsGa unit is substituted with the atomic Mn plane. The atomic structure of $M/Ga_{0.5}Mn_{0.5}As/\ Ga_{0.5}X_{0.5}As\ /Ga_{0.5}Mn_{0.5}As(001)$ (X = As, Cr, Fe and M = Fe, Cr) digital alloy multilayer consists of 14 atomic layers with one Fe

(Cr) layer on Ga-terminated surface. The first metallic plane is located on surface Ga positions and the second one in bcc geometry Fe (Cr) positions.

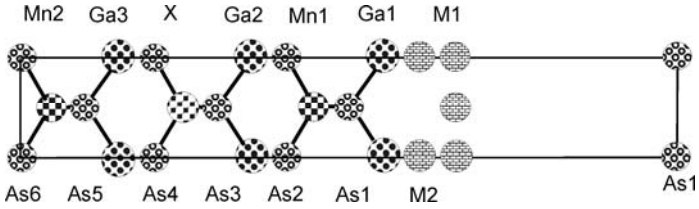

Fig. 1. The geometry of a supercell containing zinc blende 11 atomic ML, 1 ML surface metal and 8 ML vacuum, arranged along the *x*-axis

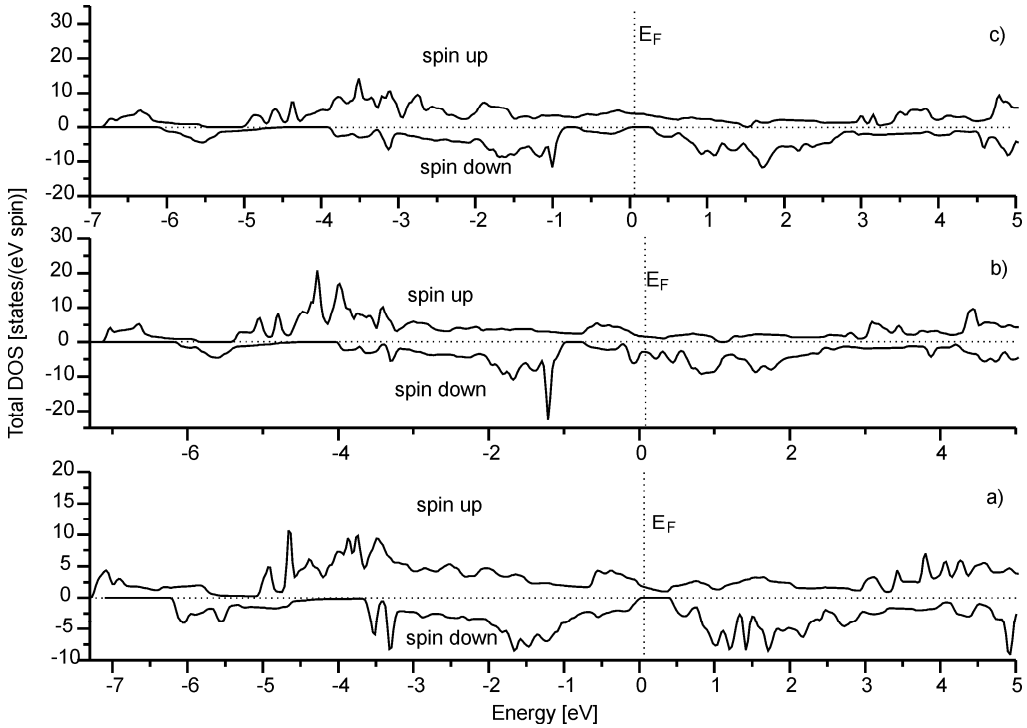

Fig. 2. The DOS functions of zinc blende $Ga_{0.5}Mn_{0.5}As/Ga_{0.5}X_{0.5}As/Ga_{0.5}Mn_{0.5}As(001)$, where atom of X dopant is: a) Ga, b) Cr, c) Fe atom

The total DOS calculations presented in Fig. 2 were performed for the $Ga_{0.5}Mn_{0.5}As$ /$Ga_{0.5}X_{0.5}As$ /$Ga_{0.5}Mn_{0.5}As(001)$ (X = Ga, Fe, Cr) multilayers which simulate DOS function (001) surface calculations. The atomic slab construction from Fig. 1 has no surface metallic monolayer. The specific semiconductor gap of ~ 0.5 eV which is characteristic of half metallic compounds is evident in Fig. 2a (X = Ga) and Fig. 2c (X = Cr) for the minority spin DOS at the Fermi energy level. The half-metallicity is destroyed with 0.5 ML of Fe on the X plane position (Fig. 1) which is evident in

Fig. 2b and the DOS for that a multilayer has a sharp semiconductor character. It was found in experiment that bilayers CrAs and GaAs can be grown in zinc blende structure by molecular epitaxy [9].

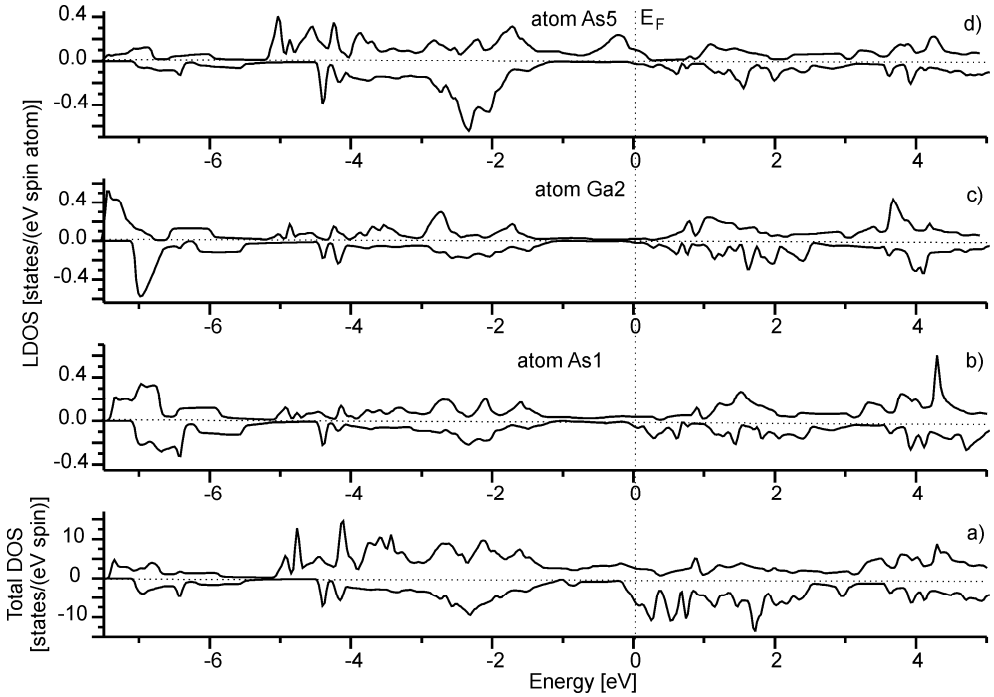

Fig. 3. The DOS functions of ZB Fe/$Ga_{0.5}Mn_{0.5}As$/GaAs/$Ga_{0.5}Mn_{0.5}As$(001):
a) total DOS, b) local DOS for As1 atom, c) the Ga2 atom LDOS, and d) the As5 atom LDOS

Figures 3a–c and 3d show total DOS and local DOS functions for the magnetic states of 1 ML Fe on the Ga-terminated surface. The LDOS are calculated in planes of As1, Ga2 and As5 atoms, and the slab construction for this atomic configuration is explained in Fig. 1. The value of lattice mismatch of α-Fe (*bcc*) which is grown epitaxially on the (001) GaAs is only 1.4% [10] and is preferable for forming heterostructures to that of δ-Fe and γ-Fe, thus we use one of Fe interface atomic plane on Ga surface positions, and one atomic plane of *bcc* Fe geometry.

A similar slab construction is used for Cr/$Ga_{0.5}Mn_{0.5}As$/ GaAs /$Ga_{0.5}Mn_{0.5}As$(001) surface DOS calculation but LDOSs are calculated for Mn1, X = Ga and Mn2 atomic planes and presented in Fig. 4.

The results of calculations of DOS functions in Fig. 3 confirm that 1 ML Fe surface layer deposited on Ga-terminated half metallic zinc blende superlattice destroys the half-metallicity of the entire multilayer. The local DOS function in As1, Ga2 and As5 planes have an evident semiconductor character. Although the minority spin total DOS function in Fig. 4 shows very small semiconductor gap at the E_F level, visibly the LDOS for ferromagnetic dopants Mn1 and Mn2 have a half-metallic character.

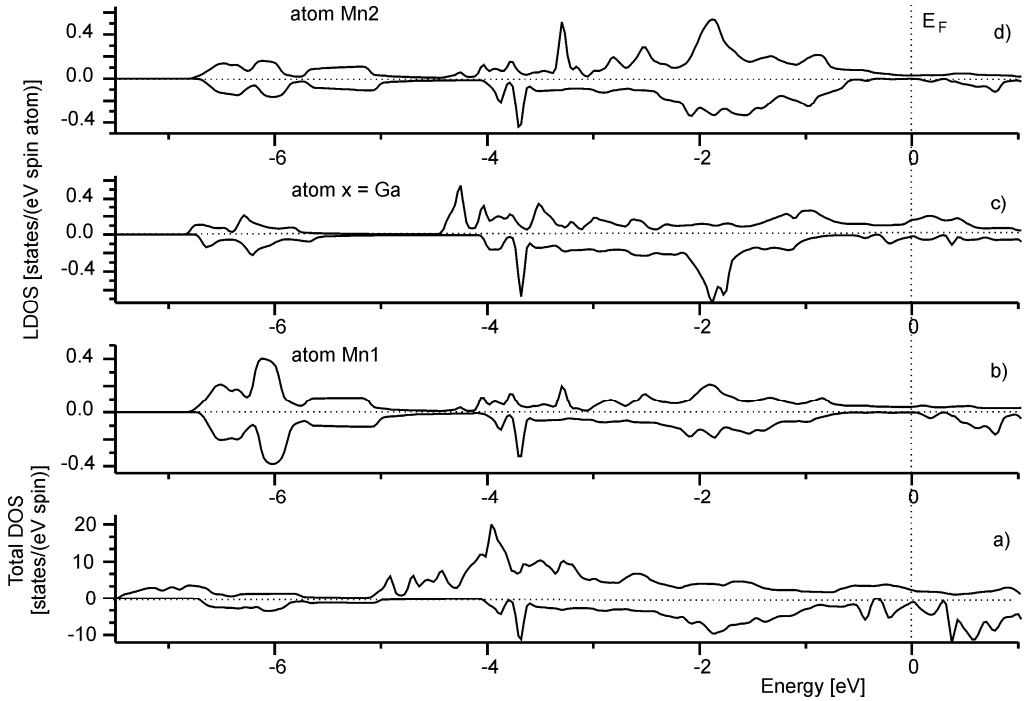

Fig. 4. The DOS functions of ZB Cr/$Ga_{0.5}Mn_{0.5}As$/GaAs/$Ga_{0.5}Mn_{0.5}As$(001):
a) total DOS, b) local DOS for Mn1 atom, c) LDOS for atom X = Ga, and d) the Mn2 atom LDOS

The calculated magnetic moments have the values in the range of (3.9–4.0)μ_B for Mn, (2.9–3.0)μ_B for Fe, and (2.8–3.1)μ_B for Cr atomic spheres in different superlattice geometries.

3. Conclusions

We investigated relaxed surfaces of zinc blende superlattices with ferromagnetic dopants (X = Fe, Cr) and M/$Ga_{0.5}Mn_{0.5}As$/ GaAs /$Ga_{0.5}Mn_{0.5}As$(001) (M = Fe, Cr) multilayers using the self-consistent FLAPW method based on the spin polarized GGA approach for total and local DOS calculations. The main results of the calculations are as follows:

- Zinc blende $Ga_{0.5}Mn_{0.5}As$/ $Ga_{0.5}X_{0.5}As$ /$Ga_{0.5}Mn_{0.5}As$(001) (X = Ga, Cr, Fe) superlattice surfaces simulated by 11 ML atomic system show half-metallic total DOS character for X = Ga and Cr, and a loss of half-metallicity for 0.5 ML of Fe in X atom position.
- The ZB heterostrucrure surface M/$Ga_{0.5}Mn_{0.5}As$/ GaAs /$Ga_{0.5}Mn_{0.5}As$(001) (M = Fe, Cr) with 1 ML metal M deposited on Ga-terminated surface loses of half-metallicity.
- Investigated ZB digital alloys demonstrate ferromagnetic arrangement of their metallic dopants (Mn, Fe, Cr).

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