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Surface half-metallicity and interfacial mixing of (Cr, Mn, Fe)VAs/GaAs(001)

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Abstract

We have investigated the magnetic and electronic properties of surface and interface for a mixed M(Ga,As) alloys with 1–2 monolayers (MLs) M(M=V, Cr, Mn, and Fe) on the GaAs(001) substrate by using first-principle calculations. We found that the surface and bulk V of zinc-blende VAs(001) half-metallic states result in diffferent lattice parameters. The surface V (or Cr) for the M-terminated zinc-blende M/As/M/GaAs(001) of 2-ML M shows a half-metallic character, while the gap in the minority-spin state of V (or Cr) in the third layer from the surface is destroyed. However, the hypothetical zinc-blende As/M/(GaM)/AsGa(001) with the surface diffusion of As atoms is found to be energetically favorable structure in the case of 2-ML M. The magnetism of V, Cr, or Mn for the 2-ML M system has the antiferromagnetic order, while for Fe it has the ferromagnetic order.

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1. Introduction

Magnetic metal/semiconductor heterostructure continues to be of intensive interest for the study of fundamental magnetism of ultrathin films and for the development of magneto-electronic devices, such as spin-dependent field effect transistors, magnetic random access memory, and magnetic reading heads [1–5]. For instance, the zinc-blende CrAs [6–9], the magnetic thin films of $Ga_{1-x}Mn_xAs$ [10–15], and a Fe thin films on the GaAs surfaces [16–20] are of current interest due to its potential for use in spin-sensitive devices.

The GaAs-based MnAs films and $Ga_{1-x}Mn_xAs$, respectively, as magnetic metal and dilute magnetic semiconductors (DMSs) appear to be promising for the spintronics applications because Mn(Ga,As) is ferromagnetic (FM) at room temperature and grows epitaxially on GaAs [12,21–23]. Zhao and coworkers have studied for the stability of the hexagonal NiAs-type MnAs on GaAs by using density-functional calculations [13]. $Ga_{1-x}Mn_xAs$ shows the FM order which is caused by the effective exchange interaction between Mn-spins via delocalized carriers [14].

Zaets et al. have proposed a conditions to grow high quality $Ga_{1-x}Cr_xAs$ films on GaAs substrates [24]. It shows that III–V DMS $Ga_{1-x}Cr_xAs$ is synthesized by low-temperature molecular beam epitaxy. The film at $T<30$ K shows a local FM ordering. It also shows that the magnetic properties of $Ga_{1-x}Cr_xAs$ sensitively depend on the growth conditions. In recent experiment, the geometric structure for a half-metallic ferromagnet zinc-blende CrAs beyond room temperature are investigated by using extended X-ray absorption fine structure measurement [6]. Shirai has theoretically studied the DMSs based on zinc-blende III–V compounds, such as V, Cr, and Mn doped GaAs by using the full-potential linearized augmented-plane-wave method [25]. It has confirmed that the FM states for zinc-blende VAs, CrAs, and MnAs is half-metallic, and is more stable than the antiferromagnetic (AF) state.

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For successful integration of MAs (M=V, Cr, Mn, and Fe atoms of 3d transition-metal) films, a detailed understanding of the growth process itself as well as the morphology and structure of the film is of crucial importance. A strong reduction of magnetization by the interfacial mixing or low spin-polarization of electrons at the Fermi level by a losing of half-metallic (i.e., the minority band presents a gap at the Fermi level) would be detrimental to the spin transport performance in spin-sensitive devices. So it is very important to reduce interfacial mixing commonly found at metal-semiconductor interfaces. The purpose of our study is to investigate the influence of intermixing on the electronic and magnetic properties for M(Ga, As) of 1–2 monolayers (MLs) M on GaAs (001). In order to simulate the interfacial intermixing, a various surface alloys of M(Ga,As) on the Ga- and As-terminated surfaces are considered.

2. Model and calculational method

The atomic structure of M(Ga, As) on GaAs(001) or AsGa(001) is modelled by a periodically repeated slab with a (1×1) surface cell. It consists of 17 and 19 atomic layers for the As- and Ga-terminated surfaces separated by six and eight layers of vacuum in the cases of 2- and 1-ML M, respectively. For 1-ML M, the surface alloys such as As/M/ (or Ga/M/), As/GaM/(or Ga/AsM/), and GaM/As/(or AsM/Ga/) on GaAs (or AsGa) are taken into account. The surface of Ga/M/AsGa(001) consists of the Ga atom, but the surface of GaM/As/GaAs(001) consists of the Ga and M atoms. This atomic structure is displayed in Fig. 1. The atomic structure for the surface difiusion of Ga or As atom in the case of 2-ML M on the substrate is Ga/M/AsM/GaAs(001), As/M/GaM/AsGa(001), and so on. Here GaM(or AsM) represents one atomic-layer, which occupies at a tetrahedral site of an empty lattice. That is, it does not mean an occupied system by 0.5 ML M. In this work, these atomic structures are called as the hypothetical zinc-blende ones.

A full-potential linear muffin-tin orbital (FPLMTO) method [26] based on the general gradient approximation (GGA) to density-functional theory with the Perdew and Wang exchange-correlation potential [27] is employed. In the determination of the lattice parameter for our slab GaAs, we use both GGA and local spin-density approximation for the comparison of lattice constants between both systems. The potential and the charge density in the crystal are treated with no shape approximation. No surface relaxation and reconstruction are allowed. Due to two empty tetrahedral-sites per layer in the zinc-blende GaAs(001), it can be included the surface lattice for the first few layers of GaAs without deforming by a strain. Spin–orbit interactions are not included. The As and Ga 3d electrons are treated as a semicore orbital and we do not use the frozen overlapped core approximation. The muffin-tin radii are chosen to be 2.24 and 2.33 a.u. for M (or Ga) and As spheres, respectively. The LMTO-basis set and charge density are expanded in terms of the spherical harmonics up to $l=6$ inside each muffin-tin sphere. The basis functions of M and Ga (or As) for the s, p and d electrons are generated with cut-off energy of $E_{\rm cut}$=197.20 (182.24), 288.32 (265.20) and 418.88 eV (387.60 eV), respectively. The charge density in the crystal has determined self-consistently by using 46 k-points corresponding to a $18\times18\times1$ grid, which insures the total energy is converged to better than 1 meV/cell.

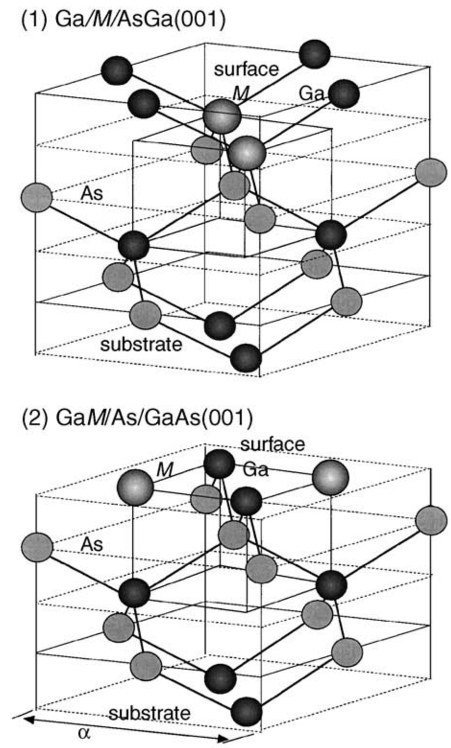

Fig. 1. Structural models for two different terminated surfaces with 1 ML M. Gray, big-, and small-black represent As, M, and Ga atoms, respectively.

3. Results and discussion

3.1. Zinc-blende VAs and V(Ga,As)

We first perform the calculations for zinc-blende VAs in order to take the equilibrium lattice constant of mixed surface alloys as illustrated in Fig. 2. The difference in total energies is calculated as a function of lattice constant for the non-magnetic and magnetic states in the zinc-blende VAs(001). It shows the energy-gain of the magnetic states compared to the non-magnetic state. The FM state is more energetically stable than the AF state for zinc-blende VAs(001). Fig. 2(b) shows the dependence for the lattice constant of the local magnetic moment at surface and bulk V sites. The local magnetic moments of bulk V site in the FM state are larger than in the AF state, while it is nearly same ones in the surface V sites. The lattice constant becomes larger than that in the non-magnetic state of each material