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Electronic structures and magnetism of As terminated zinc-blend MnAs overlayer on GaAs(001)

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1. Introduction

Since the recent report of synthesis of the zinc-blend CrAs overlayer on GaAs(001) by the molecular beam epitaxy (MBE) [1], there have been many efforts to produce various hetero-junctions for spintronics applications [2,3]. Albeit the MnAs has the other stable phases of the hexagonal NiAs-type and orthorhombic MnP-type, the zinc-blend type of MnAs, once synthesized, is predicted to be half-metallic or nearly half-metallic [4,5]. Note that Mn substituted GaAs in bulk phase is also predicted to be half-metallic [6], which is very desirable electronic structure for spintronics devices. We have recently reported a theoretical prediction that the Mn terminated zinc-blend MnAs on GaAs(001), abbreviated by MnAs/GaAs(001), is ferromagnetic semiconductor [7]. Here, we report the electronic structures and magnetism of As terminated zinc-blend MnAs on GaAs(001), abbreviated by AsMn/GaAs(001), by using the full-potential linearized augmented plane wave (FLAPW) method [8] within the generalized gradient approximation (GGA) [9].

2. Methods

We have chosen a single slab model, in which the slab is made of a two-unit-cell thickness GaAs(001) slab sandwiched by As terminated zinc-blend MnAs overlayer on each side of slab. The two dimensional lattice constant is taken to be 5.65 Å from the experiment [10]. Lattice harmonics with $l \leq 8$ were employed inside each muffin-tin sphere of radius 2.3 a.u. for all atoms, while a 13 Ry plane wave cutoff were used for the LAPW basis set. All core electrons were treated fully relativistically, while valence states were calculated scalar relativistically, without spin-orbit coupling. Self-consistency was assumed when both charge and spin density differences were less than 1.0×10^{-4} electrons/a.u.^{3} Neither the surface relaxation nor the reconstruction was considered.

3. Results and Discussions

In Fig. 1, the calculated total density of states (DOS) (a) and the atomic projected local DOS (b-g) are presented. The corresponding magnetic moments (in units of μ_B) of total and each atom are also presented in each panel. It is clearly seen that the AsMn/GaAs(001) exhibits half-metallic ferromagnetism, while MnAs/GaAs(001) is a ferromagnetic semiconductor [7]. This half-metallicity is consistent with the previous results of Mn-doped GaAs [6]. As going from the surface layers (b-c) to the central layers (f-g), the DOS of each atom displays the loss of the half-metallic character, and finally it tends to be a semiconductor, the electronic structure of bulk GaAs. The comparison of the DOSs of the As atoms (c, e, g) indicates that the half-metallic character arises from the Fermi level position located at the surface states of the spin-up bands from the As(*S*) atom. The calculated magnetic moment of the unit cell is 5.0 μ_B, and that of subsurface Mn atom is calculated to be a rather large value of 3.3 μ_B, which is, however, more than 1 μ_B smaller than that (~4.02 μ_B) of the surface Mn atom of MnAs/GaAs(001) or that (~4.4 μ_B) of Mn-doped GaAs [11].

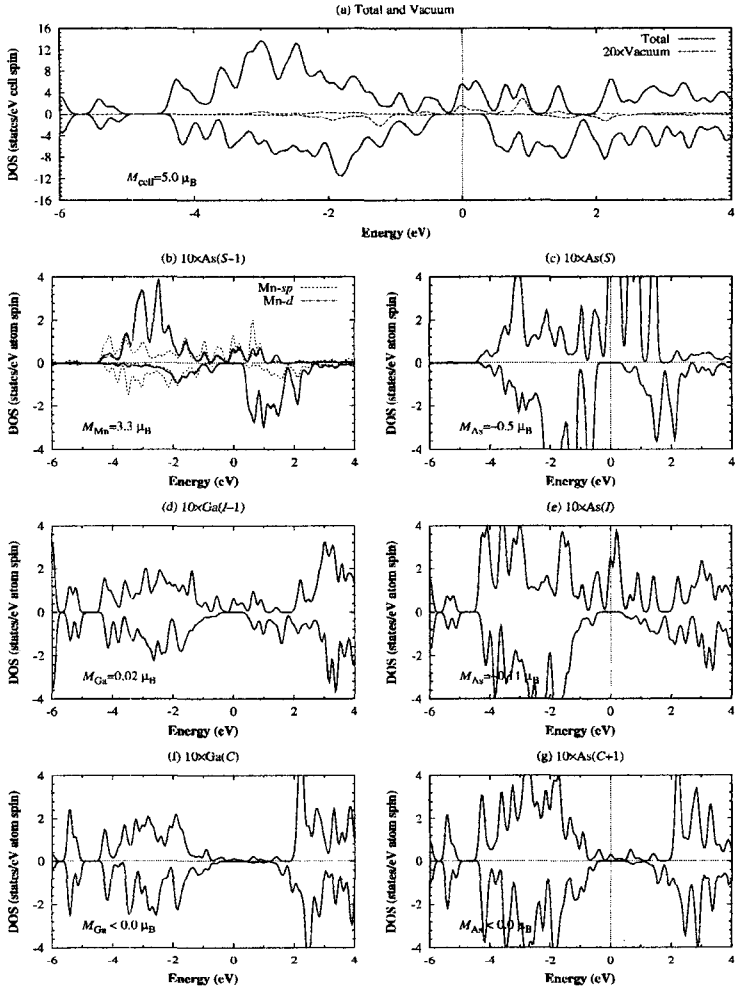

Fig. 1. Calculated spin polarized density of states of As terminated MnAs/GaAs(001) of (a) unit cell and (b-g) its atom projections. Calculated magnetic moments are also presented in each panel. Fermi level is set to zero.

4. References

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