Journal of Magnetism and Magnetic Materials 355 (2014) 295–299

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

The half metallic property and electronic structure of the Ti doped AlP systems investigated by first principle

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ARTICLE INFO

Article history:
Received 19 June 2012
Received in revised form
28 August 2013
Available online 24 December 2013

Keywords:
AlP
DFT
Half metallic
p–d Hybridization mechanism

ABSTRACT

We present numerically the ferromagnetic and spin-resolved electronic properties of Ti-doped AlP system by using first principle based on spin density functional theory. It is found that Ti impurities are spin-polarized, and it suggests a 100% polarization of the conduction carriers from the calculated band structures. Besides, the net magnetic moment of about 1 μ_B per Ti is demonstrated. The ferromagnetic state of 115.7 meV per Ti atom, lower than the anti-ferromagnetic state, is obtained by total energy calculation for both GGA and GGA+U method. And the Curie temperature, higher than 599 K, in Ti-doped AlP is predicted using mean-field approximation (MFA) theory. Both double-exchange and p–d hybridization mechanism contribute to the ferromagnetic ground state of Ti-doped AlP, but the former is dominant. Therefore, it is expected that Ti-doped AlP would be a promising dilute magnetic semiconductor for the applications in the field of Spintronics.

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1. Introduction

Spintronics, the potential second-generation electronics, focuses on the transmission of both charge and spin of electrons [1]. It has more considerable application foreground than microelectronics (the first generation electronics that only studies charges of electrons). Diluted magnetic semiconductors (DMSs) [2,3] have been confirmed to be the most promising materials, which trigger more and more research in this field. Because of the development of both the experimental and theoretical research on the DMSs, many novel researches, such as graphene based on half metallic materials and new nanostructures with Half-metallic semi-Dirac point, have been demonstrated. Half metallic materials [4,5] is one kind of novel structure materials with novel electronic and magnetic properties. A half-metal possesses unique performances which act as a conductor to electrons of one spin orientation, but as an insulator or semiconductor to those of the opposite orientation. It is well known that all half-metals are ferromagnetic (FM), but most ferromagnets materials are not half-metals. Many of half-metals are oxides, sulfides, or Heusler alloys [6] and so on. Half-metal should not be confused with semi-metal. In half-metals, the valence band for one spin orientation is partially filled while there is a gap in the density of states for the other spin orientation. This results in the conducting behavior for only electrons in the first spin orientation. Besides, in some half-metals, the majority spin channel are the conducting ones while in others the minority channel are not. Thus, half-metal material has attracted great interest for their potential applications in Spintronics.

The half metallic materials have been one of the most promising DMSs materials [7,8]. And more and more related researchers have concentrated their interest on the III-V compound DMSs [9] based on the excellent electronic and optical properties. If the spin and the charge character can be used synchronously, the III–V compound based on DMSs could be expected to be used in the next generation of Spintronics function devices [10–12]. Among the III–V compound DMSs, the investigation of Al–V compound arouses more and more research interesting. Sato et al. [13] shown that spinoadal decomposition phase in DMS offers the possibility to have high Curie temperatures (T_C) even if the magnetic exchange interaction is short ranged. Katayama-Yoshida et al. [14] have proposed materials design of high-T_C wide band-gap DMSs based on first-principles calculations by using the Korringa–Kohn–Rostoker coherent potential approximation (KKR-CPA) method. Toyoda et al. [15] have calculated the electronic structures of ZnO-based DMSs within the self interaction corrected local density approximation. Their results indicated the differences in the band gap energy, the energetic position of the Zn 3d bands, and the description of the transition-metal d bands. Parton et al. [16] indicated that the T_c was related to the band-gap of the semiconductor, while the band-gap of AlN is 6.2 eV, which was supposed to be an excellent material matrix for the DMSs. AlP is

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0304-8853/$ - see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.jmmm.2013.12.038

another important compound of Al–V compounds, and it is also a wide band-gap semiconductor [16]. The previous research on the AlP compound mainly focused on the electronic structure of the InP/AlP super lattice [3,17]. However, few research focus on the AlP matrix DMSs. Zhang et al. [18] have investigated the electronic structure and magnetic properties by the density function theory (DFT). They reported that half metallic magnetism appeared in doped AlP, but the doped atom in their studies is a kind of magnetic atom, thus it remained obscure that the magnetism is from the magnetic atom or from the interaction between atom and AlP matrix. Some other researches proposed that the ferromagnetism in semiconductors containing no magnetic atoms can be achieved [19,20]. Thus, this paper we use a nonmagnetic atom (Ti) doped AlP to make sure about the origin of magnetism.

In this paper, the electronic and magnetic properties of the nonmagnetic atom (Ti) doped AlP systems are investigated through the first-principle (FP) calculation of ultra-soft pseudopotential technology of plane wave based on the DFT. The influence of the stability of different concentration of the doped atom to the systems has been determined. The electronic structure and the half metallic properties are also illustrated through the results of the FP calculations. It is believed that our research would contribute certainly to the development of the Spintronics device.

2. Model and calculation method

In order to achieve the realistic experimental dopant concentration, we used a periodic super-cell $Al_{32}P_{32}$. And the geometrical structures of $Al_{32}P_{32}$ are optimized and compared with experimental values in order to confirm our calculations. The optimized lattice constants $a=b=c=0.5462$ nm, and the corresponding experimental values $a=b=c=0.5451$ nm, are just 0.201% difference to the experimental data. In this letter, four different doping concentrations, namely 3.175% (one doped atom in the $2\times2\times2$ super-cell), 6.25% (one doped atom in the $1\times2\times2$ super-cell), 12.5% (one doped atom in the $1\times1\times2$ super-cell) and 25% (one doped atom in the $1\times1\times1$ super-cell) (see Fig. 1(b)) were investigated. To discuss the magnetic order in the doped systems, we used two Ti atoms to replace the Al atoms in the $2\times2\times2$ super-cell, and considered the distance between the two doping atoms. We chose four different D_{Ti-Ti}, namely 3.15, 5.17, 6.18 and 7.17 Å (see the Fig. 1(a)).

The structure optimizations of Ti doped AlP and their electronic and magnetic properties are investigated by the first-principle density-functional methods, as implemented by the Vienna Ab-initio Simulation Package (VASP) [21,22]. The spin-polarized general gradient approximation (GGA) parameterized by Perdew, Burke and Ernzerhof (PBE) [23] is adopted for the exchange correlation. In choosing the computational framework, we note that the electrons can be trapped at a certain Ti atom, which would substantially increase its d-orbital occupancy. The electron occupation of Ti-3d orbital requires a careful treatment. A good example is the $LaTiO_3$, a well-known Mott insulator, with all Ti atoms in d^1 configuration. Contrary to the generalized gradient approximation (GGA), the GGA+U approach properly describes the localization nature of d electrons and shows an energy gap comparable to the experimental data. Here, a set of Coulomb (U) and exchange (J) parameters are chosen for Ti-d orbital; $U=5.0$ eV, $J=0.64$ eV [24]. The interaction between valence electrons and ion core was described by projected augmented wave (PAW) [25]. The energy cutoff for the plane-wave expansion was set to 400 eV, and the Monkhorst–Pack k-point mesh of $10\times10\times10$ was found to provide sufficient accuracy in the Brillouin-zone integration. The structural relaxation was performed using conjugate gradient algorithm and was done when the force acting on each atom is less than 0.01 eV/Å. In order to investigate the structural stability of various Ti doped AlP, their formation energy $E_{formation}$ was calculated by

$$E_{formation}=(E_{doped}-nE_{AlP}-mE_{Ti}+mE_{Al}) \quad (1)$$

where, E_{doped} and E_{AlP} are the total energies of doped and free of doped AlP, respectively; E_{Ti} is the total energy of Ti atom extracted from the Ti crystal. E_{Al} is the total energy of per atom in bulk Al.

3. Results and discussion

First, the total energies as a function of the Ti doping concentration in the ferromagnetic (FM) states were calculated as shown in Table 1. The Al atom is replaced by Ti atom in the calculated system. The results indicate that the higher the concentration is, the lower the formation energy is. And in all of the configurations, the magnetic moment of the Ti atom is between 0.833 and 0.844μ_B for GGA calculations, which the values change to 0.999 to 1.001μ_B for GGA+U calculations. Small induced magnetic moments are found in the four nearest neighboring P atoms and interstitial region, while the total magnetic moment of the calculated configuration is about 1.000μ_B. The integer value of the magnetic moment is a characteristic of half-metallic ferro-magnets [26].

Table 1
The formation energy ($E_{formation}$), the magnetic moment of the Ti atom (M_{Ti}) and the total magnetic moment of the calculated system (M_{tot}) on the concentration of the doping atom (Ti).

Doping concentration (%)	$E_{formation}$ GGA/(GGA+U) (eV)	M_{Ti} (μ_B) GGA/(GGA+U) (eV)	M_{tot} (μ_B) GGA/(GGA+U) (eV))
25.000	1.048 (1.047)	0.833 (1.049)	0.9995 (1.001)
12.500	1.072 (1.072)	0.834 (1.057)	0.9938 (1.000)
6.250	1.092 (1.094)	0.835 (1.061)	0.999 (0.999)
3.125	1.122 (1.224)	0.844 (1.090)	0.9985 (1.000)

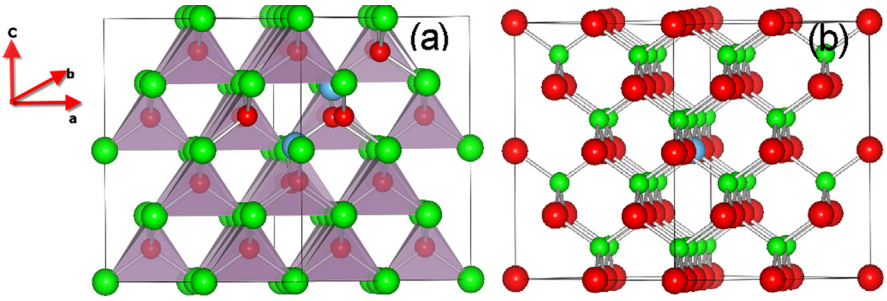

Fig. 1. The schematic illustrate the $2\times2\times2$ super-cell structure of AlP crystal, (a) denotes the configuration of two Ti atoms doped systems, (b) denotes the configuration of single Ti atom doped system. The red atoms denote the Al atoms, the green atoms denote the P atoms, and the gray atoms denote the Ti atoms. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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