Ab initio study of (Fe, Ni) doped GaAs: Magnetic, electronic properties and Faraday rotation

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ABSTRACT

The interesting diluted magnetic semiconductor (DMS), Gallium Arsenide (GaAs), was doped with the transition metals magnetic impurities: iron (Fe) and Nickel (Ni), in one hand to study the magnetic and magneto-optical properties of the material Ga(Fe, Ni) As, in the other hand to investigate the effect of the doping on the properties of this material, the calculations were performed within the spin polarized density functional theory (DFT) and generalized gradient approximation (GGA) with AKAI KKR-CPA method, the density of states (DOS) for different doping concentrations were calculated, giving the electronical properties, as well as the magnetic state and magnetic states energy, also the effect of these magnetic impurities on the Faraday rotation as magneto-optical property. Furthermore, we found the stable magnetic state for our doped material GaAs.

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1. Introduction

These last twenty years, diluted magnetic studies (DMS) have been the subject of many and considerable studies and researches leaded by different laboratories and institutes around the world, these DMSs can be divided into various categories: III-V DMSs, II-VI DMSs …, this attention has been given because of their interesting properties and applications in Spintronic devices [1,2] (II, Mn)VI diluted magnetic semiconductors (DMS) with a strongly enhanced paramagnetic behavior have been investigated [3–7]. Doped GaAs, and other DMSs of the group III–V [8,9]. The doping of these DMSs has been the key for their various applications because of the magnetism inducted by the injection of the magnetic impurities, e. g, transition metals: Mn, Ni, Fe, Co … [1,10], predicting high temperature ferromagnetism in some doped semiconductors such as GaN, ZnO, GaAs. One of the most studied and interesting DMS is GaAs, various studies has targeted this material, it has been studied from many aspects, e,g, spin-orbit interaction in GaAs wells [11], and the interface contribution of this spin-orbit interaction in the GaAs/AlGaAs [12] Udson C. Mendes et al. [13] have studied the electronic and optical properties of InGaAs wells with Mn delta doping GaAs barriers, also there are some few Ab initio calculations on GaAs, precisely, on the Mn-doped GaAs digital ferromagnetic heterostructures [14]. a remarkably high Tc about 250 K has been reported in a P-type selectively doped III-V hetero-structured composed of Mn delta-doped GaAs/p-AlGaAs [1]. There are not many theoretical studies about the Fe-doped GaAs and Ni-doped GaAs. I.R. Harris et al. [15] worked on the phase identification in Fe-doped GaAs single crystals and reported a ferromagnetic phase with a curie temperature about 100 °C, along with some

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experimental works on Fe-doping in GaAs [16], as said before, our interest comes from the lack of data concerning the magnetic and magneto-optical properties of Ga(Fe, Ni)As plus the interesting properties that the Fe doping can gives and the effect on the magneto-optical aspect, like reported in Ref. [17]. For the Ni-doping in GaAs [18], Nickel diffuses rapidly into GaAs and acts as a deep acceptor. It has often been used as a contact material on GaAs devices [19,20]. The outline of this paper is as follows. In Section 2 we present the calculation method and approximation. In section 3 we investigate and discuss the Ab initio results and then we finish by a summarizing conclusion.

2. Calculation methods

The Ab initio, first principals, calculations were executed with the AKAI-KKR-CPA code MACHIKANEYAMA2002v08 package designed and made by Akai. Korringa- Kohn-Rostoker method [21] combined with the coherent potential approximation (KKR-CPA). Based on the density functional theory (DFT), the KKR-CPA method was developed by Akai and Dedrichs to trait transition metal alloys, with the parametrization of Vosko, Wilk and Nusair (VWN) [22], e.g. in our case we have GaFeAs and GaNiAs alloys. the host material is GaAs and the transitions metals are Fe and Ni, the doping with these impurities is done randomly since the Fe and Ni atoms in each case replace and take the cation atoms (Ga) sites randomly. Therefore, we have employed the Generalized Gradient Approximations (GGA) approximation, Perdew−Wang functional, (GGA91) [22], to treat this disordered system since it is one of the most accurate and precise approximation to deal with this disorder. In our previous works we have used the local density approximation LDA approximation also [8,15].

The density of states (DOS) were calculated and plotted for both systems $Ga_{1-x}Fe_xAs$ and $Ga_{1-y}Ni_yAs$ for different doping concentrations which are the Fe, Ni magnetic impurities. To better understand the upcoming figures, the syntax "Total" represents the total density of spins up and down, located in the valence and conduction bands in the system structure. The Total density must not change from a figure to another. But the partial DOS curves will change, when varying the doping concentrations. These concentrations are x (Fe) = 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, and y (Ni) = 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07. As mentioned above, the Fe atoms are placed in the Ga sites inside the structure of GaAs. We've used in our code 300 K-point in the first Brillouin zone. Our system is a III-V direct bandgap semiconductor with a zinc blende crystal structure. See Fig. 1 with a = b = c = 5.65325 Å, as lattice constants and T_d^2-F43m as a space group. Since we have a zinc blend structure with one lattice parameter, our atoms in this system are disposed as each Ga atom is encircled by four As atoms on the corners and vice versa.

3. Results and discussion

Fig. 2 represents the Density of state (DOS) corresponding to the pure GaAs, without any doping impurities. The Fermi level is close to the conduction band and there is no impurities bands in the gap beside the symmetry between the spins up and down for both valence and band conduction, Thus our material in this case is n-type showing no magnetism as clear in the Fig. 2. It's obvious that DMSs are more interesting when there are doped with magnetic impurities which are in our case, transition metals atoms, irons (Fe) and Nickel (Ni), these transition metals contribute with their 3d bands electrons. For this purpose we proceeded by the doping of our host material, GaAs, with Fe atoms and Ni atoms separately. We have used doping concentrations from 0.01 to 0.07 for each doping impurities. We did not reach higher concentration, taking into consideration
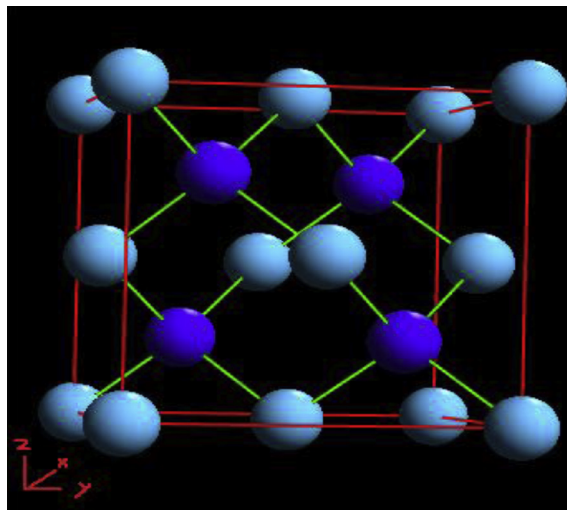

Fig. 1. GaAs zinc blende structure where Ga atoms are presented in Blue color and As atoms in purple one. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)