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Magnetoelectronic properties of Vanadium impurities co-doped (Cd, Cr)Te compound for spintronic devices: First principles calculations and Monte Carlo simulation

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ABSTRACT

We have applied the first-principles calculations to investigate magnetoelectronic properties of Vanadium impurities co-doped (Cd, Cr)Te compound for spintronic devices. The ferromagnetic (FM) nature in (Cd, Cr)Te compound co-doped with V atoms has been found, and the mechanism responsible for this behavior has been considered to be the double exchange. Moreover, the Curie-temperature calculation reveals that the stability's field of the FM-phase rises with rising both the concentration of Cr and V atoms above ambient temperature. This system presents the half-metallic character where its polarization of spin is total at the Fermi level, and its total magnetic moment is principally induced by Cr and V elements. The spin-orbit coupling (SOC) typically play an important role in the electronic structure calculations due to both the concentration of Cr and V impurities. In addition to that, our results have been confirmed by the calculation of magnetization and susceptibility using the Monte Carlo simulation.

1. Introduction

During the last few years, researchers have given a very substantial interest to dilute magnetic semiconductors (DMSs) owing to their potential application in the spintronic devices like spin valves, spin light emitting diodes, magnetic sensors, logic devices, ultra-fast optical switches, optical isolators and electrically controlled ferromagnets [1,2]. Also, some other spintronic applications have recently been intensively studied such as spin junction diodes [3,4], Giant Magnetoresistance (GMR) sensors [5,6], spin-transfer-torque magnetic random-access memory (STT-MRAM) [7,8] and solar cells [5,9]. In DMSs, a fraction of atoms is substituted by the magnetic impurities which are able to add localized magnetic moments. Thanks to this substitution, these materials not only retain the semiconducting properties according to the charge of electrons but also acquire the magnetism by means of the electron's spin. That type of doping is followed by vast series of experimental and theoretical investigations, notably DMSs based on III–V (GaAs, InAs, and GaN), II–VI (CdTe, ZnO and ZnS), IV–VI (TiO2 and SnO2) and IV (Si, Ge and Sn) semiconductors (SCs). Among the III–V semiconductors, the CdTe (Cadmium Telluride) in the zinc blende (ZB) phase is one of the most promising materials Cd-Chalcogenides (CdZ, Z = Te, Se and S) with the direct wide band gap ~1.56 eV [10]. The CdTe is used as a material for X-ray and gamma-ray detectors at ambient temperature (AT), photorefractive (PR) components, electro-optic (EO) modulators, laser windows, solar cells and substrates for epitaxial-growth of thin layers of HgCdTe (MCT) for infrared imaging systems [11].

One of the major challenges in realizing the spintronic is to synthesize ferromagnetic (FM) semiconductors that have both the semiconductor properties and the FM-behavior with the Curie-temperature (T_c) above-AT [12]. The experimental investigations reveal that Cr-doped CdTe shows ferromagnetic properties and the T_c at AT [13]. Also, Ko and Blamire found that the doping of the Chromium atoms induces ferromagnetism above-AT in CdTe bulk crystals [14,15]. In

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this context, the half-metallic (HM) ferromagnets are defined as the semiconductor spintronic materials which metallic for one-spin orientation and semiconductors or insulators for the second-spin direction. Where the spin polarization is total at the Fermi level (FL) and the dominance of the conductivity is assigned to the metallic single-spin charge carriers [16]. Since then, more and more HM-ferromagnets have been predicted theoretically using first-principles calculations in CdZ doped with various transition metals (TMs). Hardev et al. [17] found that Cr atoms doped CdZ induce ferromagnetism and retain half-metallicity with 100% spin-polarization at the FL, by using the method of the full potential linearized augmented plane wave (FPLAPW). Also, Noor et al. have shown the HM-ferromagnetic character in Cr-doped CdTe crystals using the method of the FPLAPW plus local-orbital [18]. Another theoretical study performed by Yao et al. [19] shows that the CdTe doped with Cr and V elements exhibits the HM-ferromagnetic behavior, by using the method of the plane-wave pseudopotential (PWPP).

The purpose of the present work is to study the magnetic effect of doping and co-doping CdTe with a small concentration of single and double TM impurities (Cr, V). It is found that the orbitals on Cr atoms and those of both V and Cr elements play essential roles for the magnetism with the appearance of the HM-character respectively in the $Cd_{1-x}Cr_xTe$ and $Cd_{1-2x}Cr_xV_xTe$ (x = 0.025, 0.03 and 0.04). Moreover, a special focus was devoted to the double exchange mechanism between magnetic ions, which is estimated to be the origin of FM-behavior in CdTe diluted with Cr and V impurities. Moreover, the T_c obtained with the mean-field approximation of $(Cd_{1-x}Cr_x)Te$ compound decreases with increasing the doping concentration of Cr atoms from x = 0.03 to 0.04, however that of $(Cd_{1-2x}Cr_xV_x)Te$ system increases with increasing the doping concentration of both Cr and V elements, which means that the stability's field of the FM-phase of $Cd_{1-2x}Cr_xV_xTe$ system increases with the increase of both Cr and V concentration above-AT. This result is confirmed by Monte Carlo simulation. All that make the $(Cd_{1-2x}Cr_xV_x)Te$ system a good candidate for fabricating spintronic devices.

2. Theoretical models

2.1. First-principles calculations:

The Magnetoelectronic properties of doped and co-doped CdTe based on the first-principles calculations, have been studied, with the local density approximation and using the KKR-method united with the coherent potential approximation (LDA-KKR-CPA) [20], within the Moruzzi, Janak and Williams parameterization (MJW) [21]. The LDA-KKR-CPA method is especially adapted in order to study disorder systems as like DMSs.

In this study, the calculations are performed using the MACHIKANEYAMA2002v08-package designed and made by Akai [22]. The relativistic effect has been taken into account by employing the scalar relativistic approximation (SRA), as well as the crystal potential is approximated by Muffin tin approach. In order to treat our compound, we have used up to 500 K-points in the irreducible part of the first-Brillouin zone. We have obtained the optimized lattice parameter for CdTe, $(Cd_{1-x}Cr_x)Te$ and $(Cd_{1-2x}Cr_xV_x)Te$ by performing the calculated values of total energy as a function of the lattice parameter, we have found that the minimum energies of all these materials are around 6.48 Å which shows a good agreement with experimental data (a = 6.486 Å) [23]. The CdTe compound exhibits the ZB-structure with the space group F43m, which four Cd atoms are positioned at (0 0 0); (0 0.5 0.5); (0.5 0 0.5); (0.5 0.5 0) and four Te atoms at (0.25 0.25 0.25); (0.25 0.75 0.75); (0.75 0.25 0.75); (0.75 0.75 0.25). To ameliorate our calculations, two additional empty spheres representing atomic inter sites are placed at (0.5 0.5 0.5); (0.75 0.75 0.75). The electronic configurations for Cd (Z = 48), Te (Z = 52), V (Z = 23) and Cr (Z = 24) are respectively [Kr] $4d^{10}5s^2$, [Kr] $4d^{10}5s^25p^4$, [Ar] $3d^34s^2$ and [Ar] $3d^54s^1$.

We calculate the energy difference $\Delta E = E_{DLM} - E_{FM}$ between the disordered local moment (DLM) state and the FM-state so as to disclose the magnetic phase stability in DMSs. When ΔE is positive, the system is stable. Otherwise, we have a disordered local moment.

Founded on the mean-field (MF) approximation, the T_c is calculated in terms of the impurities' concentration (c), by using the following equation:

$$k_B T_c = \frac{2}{3}\frac{E_{DLM} - E_{FM}}{c} \quad (1)$$

where k_B is the Boltzmann's constant.

2.2. Monte Carlo simulation

While first-principles calculations donate the fundamental electronic aspects of the system, it is unable to describe the systems at non-zero temperatures. In this section, we prolong the zero temperature using Monte Carlo (MC) simulation [24] founded on the Heat-Bath algorithm (HBA) in order to study the total magnetization and the susceptibility of $(Cd_{1-2x}Cr_xV_x)Te$ system. The capacity to precisely treat DMS systems by the Ising model is mainly due to the weak concentration of the magnetic impurities in the host-SCs and the low interaction moments.

The system's Hamiltonian is given by

$$H = -J_{Cr-Cr}\sum_{ij} S^{Cr}_{i,z}S^{Cr}_{j,z} - J_{V-V}\sum_{nm} S^{V}_{n,z}S^{V}_{m,z} - J_{Cr-V}\sum_{in} S^{Cr}_{i,z}S^{V}_{n,z}, \quad (2)$$

where, $J_{Cr\text{-}Cr}$ and $J_{V\text{-}V}$ are the parameters of the exchange interaction between two close-neighbor (Cr-Cr) impurities and the (V-V) impurities, respectively, and $J_{Cr\text{-}V}$ is the exchange interaction parameter between two close-neighbor Cr impurity and the V impurity. $S^{Cr}_{i,z}$ spins receive the values 0, ± 1 and ± 2 at every site-i and $S^{V}_{n,z}$ spins receive the values 0 and ± 1 at every site-n of $Cd_{1-2x}Cr_xV_xTe$ Ising model. The summation index < ij > , < nm > and < in > indicate a summation

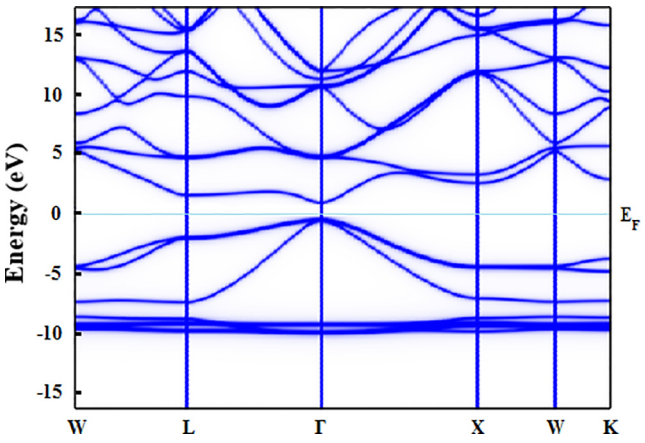

Fig. 1. The band structure of CdTe.