



The spin effect in zinc-blende $\text{Cd}_{0.5}\text{Mn}_{0.5}\text{Te}$ and $\text{Zn}_{0.5}\text{Mn}_{0.5}\text{Te}$ diluted magnetic semiconductors: FP-LAPW study

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ABSTRACT

In this work we use the full potential linearized augmented plane wave (FPLAPW) method within the local spin density approximation. Our goal is to study the structural, electronic and magnetic properties of the ferromagnetic CdMnTe and ZnMnTe semiconductors alloys in its ordered chalcopyrite phases (50% of Mn). We have investigated the lattice parameters, bulk moduli, band structures, total and partial densities of states. The determined exchange constants $N_0\alpha$ (conduction band) and $N_0\beta$ (valence band) somewhat agree with a typical magneto-optical experiment. In these systems the s(p)-d exchange interaction between free electrons (holes) and localized magnetic moments plays an important role for their characteristic properties. Our results show that the localization of the Mn spin-majority states are positioned near the top of the valence band and strongly hybridized with it. Furthermore, calculations predict that the p-d hybridization reduces the local magnetic moment of Mn from its free space of 5–4.32 μ_B for $\text{Cd}_{0.5}\text{Mn}_{0.5}\text{Te}$ and 4.23 μ_B for $\text{Zn}_{0.5}\text{Mn}_{0.5}\text{Te}$.

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1. Introduction

The Mn doped II–IV based semimagnetic semiconductors or diluted magnetic semiconductors (DMSs) and related nanostructures belong to an attractive materials owing to their unique properties and because of new possibilities of application in spintronic devices [1,2]. However, the recent developments in crystal growth and especially in molecular beam epitaxy (MBE) allow now zinc-blende (ZB) structure crystals of CdMnTe , ZnMnTe and ZnMnSe to be grown in the entire composition range $0 < x < 1$. As a result of the tunability of the lattice parameters, these materials are excellent candidates for growing quantum wells and superlattices that have interesting magnetic and magneto-optical properties.

Experimentally, CdMnTe is the most thoroughly studied compound. The above interest has extended into the area of thin film technology, and consequently there has been a number of reports of the epitaxial growth of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ [3–7]. In contrast, only some researchers have reported on the energy band gap, structural characteristics, Raman scattering, magnetic properties and magneto-optical properties in bulk $\text{Zn}_{1-x}\text{Mn}_x\text{Te}$ [2,8–13], and only a few reports on $\text{Zn}_{1-x}\text{Mn}_x\text{Te}$ epilayers [14–20].

Both DMSs $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ and $\text{Zn}_{1-x}\text{Mn}_x\text{Te}$ exhibit ZB structures at composition $x < 0.70$ and $x < 0.86$, respectively. Above these compositions, multiphase structures prevail for $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ alloy, and NiAs structures for $\text{Zn}_{1-x}\text{Mn}_x\text{Te}$ alloy [8], whereas, their binary CdTe and ZnTe have the ZB structure and the bulk MnTe has the NiAs (hexagonal) structure [21]. In particular, Mn-based II–VI DMSs are stable in the antiferromagnetic phase; consequently, it becomes necessary to make a codoping by p-type carrier-induced ferromagnetism. Recently, using the MBE techniques and the azote(N)element as codoping, carrier-induced ferromagnetism has been demonstrated for p-type CdMnTe quantum wells (QWs) [22] and p-type ZnMnTe [23]. Curie temperatures of 1.5 and 3 K, respectively, have been achieved.

Theoretically, early works for $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ have been performed by Larson et al. [24] using the augmented spherical-wave (ASW) method, Hass et al. [25] using the empirical tight-binding (ETB) method and Wei and Zunger [26] using full relativistic linear augmented plane-wave (FLAPW) method. The LAPW calculations reported by Wei and Zunger have briefly reported on the results of fully self-consistent calculations of the ground-state properties of ferro- and antiferromagnetic cubic MnTe and presented the first picture of the electronic structure of ferromagnetic CdMnTe_2 . Recently, most of the published ab initio studies performed for TM-doped Zn-based II–VI compounds (i.e. TM is the transition metal) have been focused on the research of new DMSs having high T_C [27,28]. Few of them have been concerned to investigate

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the electronic structure [29–31]. The study of the structural properties of ZnTe, MnTe, and $\text{Mn}_{1-x}\text{Zn}_x\text{Te}$ alloy with ZB, NiAs, and Wurtzite (WZ) phases by PWSCF ab initio calculations have been reported by Gonzalez Szwacki et al. [32]. Their calculations predict that the dominant phases for $x < 0.25$ and $x > 0.25$ are NiAs and ZB, respectively, and that the WZ phase is higher in energy than the ZB phase by 0.04 eV for all compositions.

In this work, our interest was to look for common trends and differences in electronic and magnetic structure of ferromagnetic $\text{Cd}_{0.5}\text{Mn}_{0.5}\text{Te}$ and $\text{Zn}_{0.5}\text{Mn}_{0.5}\text{Te}$ in its ordered chalcopyrite phase. Since we focus on the magnetic properties, we pay particular attention to the exchange constants, which are essentially constant parameters. The purpose in all of these calculations has been to provide a fundamental understanding of the ground state properties of both ferromagnetic $\text{Cd}_{0.5}\text{Mn}_{0.5}\text{Te}$ and $\text{Zn}_{0.5}\text{Mn}_{0.5}\text{Te}$ DMS alloys.

2. Details of calculations

The equilibrium structural parameters were calculated using the Vienna package WIEN2K [33]. This is an implementation of a hybrid full-potential (linear) augmented plane-wave plus local orbitals (L/APW+lo) method within the density-functional theory [34,35]. This new approach is shown to reproduce the accurate results of the LAPW method, but using a smaller basis set size. Due to the smaller basis set and faster matrix set up, APW+lo offers a shorter run-time and uses less memory than LAPW. The effects of using APW+lo are greatest for calculations with a large ratio of basis functions to atoms, e.g. for open crystal structures, surfaces and molecules on surfaces [36].

The APW+lo method expands the Kohn–Sham orbitals in atomic like orbitals inside the atomic muffin-tin (MT) spheres and plane waves in the interstitial region. The details of the method have been described in the literature [36–38]. The basis set inside each MT sphere is split into core and valence subsets. The core states are treated within the spherical part of the potential only and are assumed to have a spherically symmetric charge density totally confined inside the MT spheres. The valence part is treated within a potential expanded into spherical harmonics up to $l=4$. The valence wave functions inside the spheres are expanded up to $l=10$. A plane-wave expansion with $R_{\text{MT}} \times K_{\text{MAX}}$ equal to 8, and k sampling with a $6 \times 6 \times 3$ k -points mesh in the full Brillouin zone turns out to be satisfactory. All of the calculations were carried out at the theoretical equilibrium lattice constants.

We take the Perdew–Wang local spin density approximation (LSDA) [39]. The self-consistent calculations are considered to be converged only when the calculated total energy of the crystal converged to less than 1 mRyd. The choice of the particular (and different) muffin-tin (MT) radii for the various atoms in the compounds shows small differences that do not affect our results. We compute lattice constants and bulk modulus by fitting the total energy versus volume according to the Murnaghan's equation of state [40].

3. Results and discussion

3.1. Structural properties

In order to simulate the ordered ZB structure with 50% of Mn, we consider a model based on an eight-atoms supercell. As we know, the supercell approach is used to restrict the dopant concentration to a small value, which is of interest for studying

the magnetic properties of the system, without altering the original underlying lattice structure. Since the dopant concentration is of 50% (i.e. high composition) we have used a small supercell with space group $\bar{1}42d$ (D_{2d}^{12}) instead of using a large supercell. Indeed the effect of a small supercell on magnetic properties is discussed in Section 3.5.

The XMnTe_2 compounds studied here are in the tetragonal chalcopyrite structure. This structure can be described by three structural parameters: the lattice constant a , the tetragonal ratio $\eta = c/2a$, and the anion displacement u . The u parameter is related to the two types of anion–cation bond lengths by

$$u = \frac{1}{4} + \frac{R_{\text{X-Te}}^2 - R_{\text{Mn-Te}}^2}{a^2}$$

where $R_{\text{X-Te}}$ and $R_{\text{Mn-Te}}$ are the bond lengths of X–Te and Mn–Te, respectively. In the ideal structure which is our case, the bond lengths X–Te and Mn–Te are equal (i.e. $u = 0.25$ and $\eta = 1$).

The calculated structural parameters of ZB binary CdTe, and ZnTe and ternary CdMnTe, and ZnMnTe alloys are listed in Table 1.

3.2. Band structures and density of states

Our calculations of the electronic properties (band structure and density of state) are performed at the equilibrium lattice parameters for the ZB CdMnTe and ZnMnTe with 50% of Mn in the chalcopyrite structure.

Fig. 1 describes schematically how the band structure of the chalcopyrites evolves from the ZB analogs [41]. For direct-gap ZB semiconductors with T_d symmetry, such as for CdTe and ZnTe, the valence band maximum (VBM) is a bonding triply degenerate Γ_{15} state. In chalcopyrites with the lower D_{2d} symmetry, the triply degenerate Γ_{15} VBM state splits into nondegenerate Γ_{4v} and doubly degenerate Γ_{5v} states [41,42]. The crystal field splitting $\Delta_{\text{CF}} = E(\Gamma_{5v}) - E(\Gamma_{4v})$ is defined as positive if the Γ_{5v} states lie above the Γ_{4v} states.

The plots of the spin polarized band structures of these DMSs are presented in Figs. 2 and 3 for CdMnTe and ZnMnTe, respectively. The calculated energy gaps at high symmetry points deduced from spin-up band structure, and the crystal field Δ_{CF} values for both DMSs are reported in Table 2. Therefore our results predict a smaller spin-up direct band gap (0.61 eV) for CdMnTe and (0.77 eV) for ZnMnTe than the spin-down direct band gap (1.72 eV) for CdMnTe and (1.73 eV) for ZnMnTe. Furthermore, from Figs. 2 and 3, the d states with e_g symmetry were only slightly broadened by hybridization, while t_{2g} states were strongly hybridized with the Te-5p states. They contributed to the density

Table 1

Calculated LDA lattice constants a (in Å), bulk modulus B and the derivative of the bulk B' of the ferromagnetic CdMnTe and ZnMnTe with 50% of Mn.

		a (Å)	B (GPa)	B'
CdMnTe	Present ^a	6.32	49.94	7.46
	FP-LAPW [26] ^b	6.37		
	Exp. [46]	6.39		
CdTe	Present	6.424	44.38	4.43
	FP-LAPW [26]	6.46		
	FP-LAPW [48]	6.421	46.18	4.60
	Exp. [46]	6.481	44.50	6.40
ZnMnTe	Present ^a	6.11	54.55	6.61
ZnTe	Present	6.011	56.77	4.19
	FP-LAPW [48]	6.027	55.67	4.90
	Exp. [49]	6.089	50.90	5.04

We assumed $\eta = c/2a = 1$, $u = 0.25$.

^a Chalcopyrite phase (space group D_{2d}^{12}).

^b CuAu-I phase (space group D_{2d}^{12}).

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