Journal of Magnetism and Magnetic Materials 351 (2014) 60–64

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

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

Density functional studies of magneto-optic properties of CdCoS

Rashid Iqbal [a], Imad Khan [a,*], H.A. Rahnamaye Aliabad [b], Zahid Ali [a], Iftikhar Ahmad [a]

[a] Department of Physics, University of Malakand, Chakdara, Pakistan
[b] Department of Physics, Hakim Sabzevari University, Sabzevar, Iran

ARTICLE INFO

Article history:
Received 19 August 2013
Received in revised form
5 September 2013
Available online 28 September 2013

Keywords:
Optical material
Chalcogenides
Electronic band profile
Magnetism
Solar cell

ABSTRACT

Density functional calculations are performed to investigate the structural, electronic, magnetic and optical properties of $Cd_{1-x}Co_xS$ ($0 \le x \le 0.75$) in cubic zinc-blende structure. Accurate exchange potential modified Becke and Johnson (mBJ) within the FP-FLAPW method has been used in the calculations. Lattice constant of the alloy decreases while band gap first decreased and then increased with increased in Co concentration. The decrease in the band gap of CdS substituted Co 25% is because of the exchange interaction between Co-3d and S-3p state. The ferromagnetic nature of material is due the spin polarization of Co-3d state and the magnetization of the compound is increased with increased in Co concentration. The band gap energy varies mostly in visible region of the electromagnetic spectrum; therefore the material is precious for solar cell application. The optical properties like dielectric constant, index of refraction and reflectivity are also calculated.

1. Introduction

The energy consumption rate of the world is continuously increasing and will reach to 30 Terawatt years (TWyr) in 2050 [1]. Looking to this exponential increase in energy consumption, the world will soon reaches to an energy desert. To handle this disastrous situation there seems only few energy sources which can meet this huge demand. Due to the environmental friendly nature of solar energy, it is the most favorable energy source. The material scientists already have stepped forward to exploit this infinite source of energy. Different techniques such as photochemical, photothermal and photoelectrical conversion are being used to utilize the solar energy. Presently solar energy is cost effective and contributes only 1% of the world requirements.

For solar energy conversion, efficient and cheap materials are most important in the fabrication of photonic cell. Most of chalcogenides are renowned as effective materials for solar energy conversion [2–4]. In this regard CdCoS is one of the most favorable chalchogenide materials for solar cell applications. This compound has also potential applications in optical window layers, photocells, antireflective coating material for poultry houses, temperature sensors and optical waveguides [5–9].

The compound has been sensitized experimentally by different techniques. Thin films of $Cd_{1-x}Co_xS$ ($x=0$, 0.025, and 0.05) were deposited on glass substrates by the thermal evaporation method [10]. Chandramohan et al. [11] studied structural, optical, vibrational and morphological properties of Co-doped CdS thin films (from 0.34% to 10.8%) prepared by the ion implantation method. It is also deposited on microscopic glass substrate using the chemical bath deposition (CBD) technique [12,13]. $Cd_{1-x}Co_xS$ ($0 \le x \le 0.5$) thin films were deposited by liquid phase chemical bath deposition (LPCBD) process [14]. Structural, optical and magnetic properties of CdS thin films with the addition of Co prepared by (i) spray pyrolysis of $Cd_{1-x}Co_xS$ ($x \leqslant 0.10$) thin films and (ii) Co diffusion doped CdS films were investigated [15]. Sathyamoorthy et al. [16] synthesized $Cd_{1-x}Co_xS$, nanoclusters for different Co concentrations ($x=0.10$, 0.20 and 0.30) by the surfactant-assisted method and investigated their structural, electronic, optical and magnetic properties. Saravanan et al. [17] used the aqueous chemical co-precipitation method to synthesis and studied different physical properties of CdCoS at 2, 4, 6% of Co concentration, whereas Saeed et al. [18] studied structural, electronic and magnetic properties $Cd_{1-x}Co_xS$ ($x=0.25$, 0.50 and 0.75) using the density functional theory.

The above mentioned experimental results reveal that the alloy (for wide range of Co concentration i.e. 50%) is a wide band gap ferromagnetic semiconductor, while the previous theoretical results [18] show that the material is half metal for the whole range of Co concentration. To provide accurate and precise theoretical foundation to the experimental results, it is necessary to revisit the reported results with efficient model. In the present study the structural, electronic, magnetic and optical properties of $Cd_{1-x}Co_xS$ ($0 \le x \le 0.75$) are investigated using first principle calculations with modified Becke and Johnson exchange potential (mBJ). The present theoretical study confirms the wide band gap and ferromagnetic nature of the compound.

2. Computational detail

The full potential linearized augmented plane wave (FPLAPW) method as implemented in the Wien2k package [19] is used in the

* Corresponding author. Tel.: +92 344 6643723.
E-mail address: Imadkhan723@gmail.com (I. Khan).

0304-8853/$ - see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.jmmm.2013.09.016

present calculations. For the structural properties the electrons exchange-correlation energy is described by generalized gradient approximation (GGA), where for the calculation of band gaps and optical properties modified Becke–Johnson (mBJ) exchange potential [20] is used. mBJ exchange is quite successful in the calculation of band gaps of the strongly electron systems especially II–VI semiconductors [21–23].

Basis functions are expanded as combination of spherical harmonic functions inside non-overlapping spheres around the atomic sites (muffin-tin) and in Fourier series in the interstitial region. For the wave function expansion inside the atomic spheres, the value of l is confined to $l_{max}=10$, and for the interstitial non-spherical part $l_{max}=6$. The wave functions in the interstitial region were expanded in plane waves with a cutoff of $k_{max}=8/R_{mt}$ (R_{mt} is the average radius of the muffin-tin spheres). The brillouin zone integration is performed using a mesh of 2000k-points, and convergence is checked through self-consistency.

3. Result and discussion

3.1. Structural properties

It is evident from the experimental [16,24] and theoretical results [18] that the alloy $Cd_{1-x}Co_xS$ exhibit ferromagnetic nature at various Co concentrations. In the calculations the alloys are modeled at various Co compositions in the step of 0.25 in zinc-blende ferromagnetic phase. Each unit cell is optimized by minimizing total energy with respect to cell volume and the calculated lattice constants and bulk moduli are obtained by fitting the total energy versus unit cell volume to the Murnaghan's equation of state [25]. The calculated lattice constants and bulk moduli are compared with available experimental and theoretical results in Table 1. Our calculated results are in agreement with the experimental and theoretical results. The table reveals that the lattice constant decreases and bulk modulus increases with increasing Co concentration. This decrease in lattice constant and increase in bulk modulus is also shown against concentration x in Fig. 1. It is obvious from the plot that both the quantities varies non-linearly with Co concentration and deviate largely from the Vegard's law. The decrease in lattice constant is due to the substitution of smaller ion Co^{+2} instead of Cd^{+2}.

Table 1
Calculated lattice constant a (Å), bulk modulus B (GPa) and band gap $E_g^{\Gamma-\Gamma}$ (eV) in majority spin (up) channel for $Cd_xCo_{1-x}S$ ($x=0$, 25, 0.50, and 0.75) compared to other calculations and experiments.

x	Experimental	Theoretical	
		Present	Other
0.0			
a	5.82[a]	5.83	5.83[b]
B	62[a]	58.497	72.27[b]
E_g	2.55, 2.4[c]	2.56	2.56[b]
0.25			
a		5.77	5.63[d]
B		68.2068	73.1113[d]
E_g		1.6	1.1[d]
0.50			
a		5.53	5.54[d]
B		74.4446	69.3983[d]
E_g	1.94[e]	1.82	1.3[d]
0.75			
a		5.38	5.25[d]
B		97.8422	76.0669[d]
E_g		2.22	1.5[d]

[a] Ref. [27].
[b] Ref. [28].
[c] Ref. [26].
[d] Ref. [18].
[e] Ref. [14].

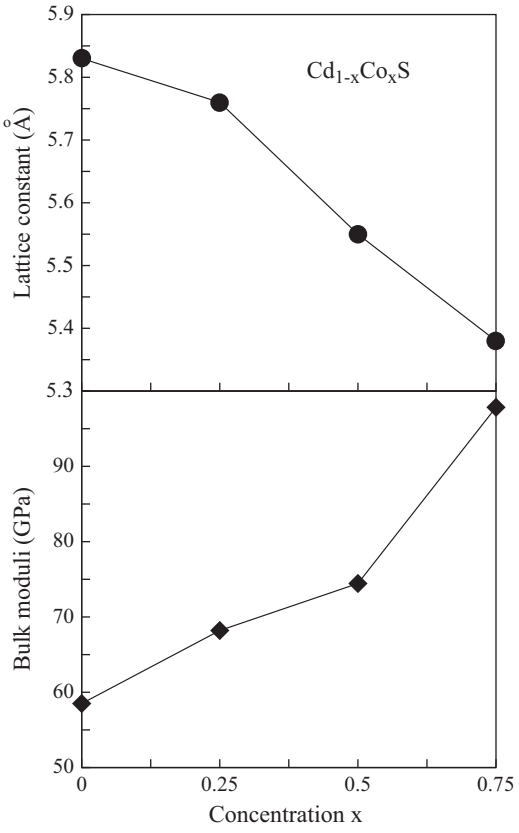

Fig. 1. Variation of lattice constant and bulk modulus of with Co concentration.

3.2. Electronic properties

To identify efficient materials for optoelectronic, magneto-optic and electromagnetic devices, the knowledge of band gap is important [28]. The previous local density approximation calculation [18] of band gap show that the alloys $Cd_{1-x}Co_xS$ ($x=0.25$, 0.50, and 0.75) are half metallic having semiconducting nature in spin up and metallic nature in spin down state, which are consist with the experimental results. Experimentally the alloys $Cd_{1-x}Co_xS$ ($0\le x\le 0.75$) are wide and direct band materials and find their applications in optoelectronic devices [14]. Therefore, to provide accurate theoretical foundation to the experimental results, the band gap calculation are carried out using efficient potential mBJ, which show that the material is semiconducting in nature. The calculated spin polarized band structures of $Cd_{1-x}Co_xS$ ($x=0$, 0.25, 0.50, and 0.75) are presented in Fig. 2a–f. From the figure it is clear that in spin up channel (majority spin) the alloy has direct band gap (Γ-symmetry) nature for the whole range of concentration, while in case of spin down state except at $x=0.25$ indirect band gap nature (Γ–M-symmetry) is observed. The calculated band gaps are compared with the available theoretical and experimental results in Table 1. From the table it is clear that the band gap of the binary compound (CdS) is 2.56 eV which in agreement with the experimental. The band gap of ternary decreases at $x=0.25$, this reduction is due p-d exchange interactions between the host material s–p band electrons and the localized d electrons of the Co ions at the top of valence band. Our calculated band gap of $Cd_{0.50}Co_{0.50}S$ is found in agreement with the experimental data [14], which the accuracy of the