Physica B 406 (2011) 2509–2514

Contents lists available at ScienceDirect

Physica B

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

Bandgap engineering of $Cd_{1-x}Sr_xO$

I. Khan, Iftikhar Ahmad*, B. Amin, G. Murtaza, Z. Ali

Materials Modeling Laboratory, Department of Physics, Hazara University, Mansehra, Pakistan

ARTICLE INFO

Article history:
Received 10 December 2010
Received in revised form
16 March 2011
Accepted 17 March 2011
Available online 13 April 2011

Keywords:
Optoelectronic
Bandgap engineering
CdO:Sr

ABSTRACT

Structural, electronic and optical properties of $Cd_{1-x}Sr_xO$ ($0 \leq x \leq 1$) are calculated for the first time using density functional theory. Our results show that these properties are strongly dependent on x. The bond between Cd and O is partially covalent and the covalent nature of the bond decreases as the concentration of Sr increases from 0% to 100%. It is found that $Cd_{1-x}Sr_xO$ is an indirect bandgap compound for the entire range of x and the bandgap of the alloy increases from 0.85 to 6.00 eV with the increase in Sr concentration. Frequency dependent dielectric functions $\varepsilon_1(\omega)$, $\varepsilon_2(\omega)$, refractive index $n(\omega)$ and absorption coefficient $\alpha(\omega)$ are also calculated and discussed in detail. The peak value of refractive indices shifts to higher energy regions with the increase in Sr. The striking feature of these alloys is that $Cd_{0.5}Sr_{0.5}O$ is an anisotropic material. The larger value of the extraordinary refractive index confirms that the material is positive birefringence crystal. The present comprehensive theoretical study of the optoelectronic properties of the material predicts that it can be effectively used in optoelectronic applications in the wide range of spectrum; IR, visible and UV.

1. Introduction

The group II–VI semiconductors have been extensively studied due to their effective use in optoelectronic industry. These compounds are commonly used in many established commercial electronic and optoelectronic devices operating in blue to ultraviolet spectral regions [1–5]. Optically transparent and electrically conductive nature of CdO makes it an important member of the group. Its industrial applications are not limited to solar cells, transparent electrodes, ohmic contacts to LEDs, smart windows, optical communications, flat panel displays, photo-transistors, photovoltaics, gas sensors, low-emissive windows and thin-film resistors [6–12] but it is also efficiently used as a high reflective compound in the infrared region while high transparent material in the visible region [10]. Bandgap of CdO is 0.85 eV, while strontia (SrO) is an insulator with bandgap of 5.71 eV [13,14]. Strontia is used as a catalyst in chemical engineering [15] and is also used in cathode ray tubes for the blocking of X-ray emission.

Knowledge of bandgap engineering and optical properties of semiconducting compounds is a promising field of study for the design of optoelectronic and photonic devices. A systematic change in the bandgap of a binary material can be achieved by the partial substitution of anion or cation of a crystal by an element of desirable properties.

In the present theoretical work bandgap of rock salt CdO is varied systematically by alloying with Sr. In order to investigate optoelectronic nature of these alloys their structural, electronic and optical properties are calculated. All calculations are based on density functional full potential linearized augmented plane wave (FP-LAPW) method with Wu–Cohen generalized gradient approximation (GGA).

2. Theory and calculation

The calculations are performed by FP-LAPW approach within the framework of density functional theory (DFT). The exchange-correlation energy of electrons is described by GGA. The GGA functional form Wu–Cohen is used within the wien2k package [16].

In the full potential scheme both, the potential and charge density, are expanded into two different bases. Within the atomic sphere the potential is expanded in spherical harmonics while outside the sphere (interstitial region) it is expanded in plane wave basis. The expanded potentials are

$$V(r) = \begin{cases} \sum\limits_{lm} V_{lm}(r) Y_{lm}(r) & \text{(a)} \\ \sum\limits_{k} V_k e^{ikr} & \text{(b)} \end{cases} \tag{1}$$

Inside the sphere potential is spherically symmetric while outside the sphere it is constant. R_{MT} is chosen in such a way that there is no charge leakage from the core and hence total energy convergence is ensured. R_{MT} values of 2.41, 2.33 and

---

* Corresponding author.
E-mail address: ahma5532@gmail.com (I. Ahmad).

0921-4526/$ - see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.physb.2011.03.042

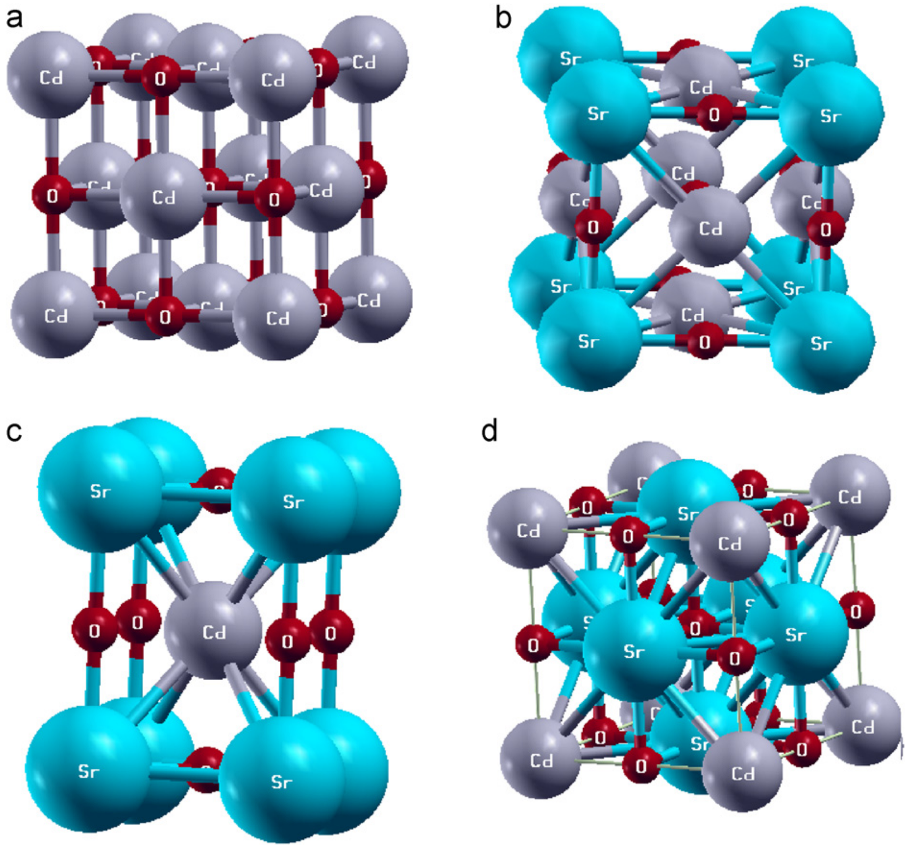

Fig. 1. Crystal structure of (a) CdO, (b) $Cd_{0.75}Sr_{0.25}O$, (c) $Cd_{0.50}Sr_{0.50}O$ and (d) $Cd_{0.25}Sr_{0.75}O$.

Table 1
Lattice constants of $Cd_{1-x}Sr_xO$ $(0 \leq x \leq 1)$ compared with experimental results, Vegard's law and other theoretical calculations.

Lattice constants, *a* and *c* (Å) *x*	This work	Experiment	Vegard's law	Other calculation
0	4.69	4.689 [11]		4.664 [14]
0.25	4.80		4.79	
0.50	3.49, 5.56		4.89	
0.75	5.00		4.99	
1	5.10	5.159 [11]		5.093 [14]

2.19 a.u. are used for Cd, Sr and O, respectively. For wave function in the interstitial region the plane wave cut-off value of $K_{max}=7/R_{MT}$ was taken. The Monkhorst–Pack grids *k*-points from $5\times5\times5$ up to $43\times43\times43$ are used in the Brillouin zone integration and convergence was checked through self-consistency. The convergence was ensured for less than 1 mRy/a.u.

Structural properties of $Cd_{1-x}Sr_xO$ are calculated using Murnaghan's equation of state [17]:

$$E(V)=E_0+\frac{B_0V}{B'_0}\left(\frac{(V_0/V)^{B'_0}}{B'_0-1}+1\right)-\frac{B_0V_0}{B'_0-1} \qquad (2)$$

where E_0 is the total energy of the supercell, V_0 is the unit volume, B_0 is the bulk modulus at zero pressure and B'_0 is the derivative of bulk modulus with pressure.

Optical properties of $Cd_{1-x}Sr_xO$ are calculated using a fine *k* mesh of 3500 points for the present calculation. The dielectric function of a crystal depends on the electronic band structure and its investigation by optical spectroscopy is a powerful tool in the determination of the overall optical behavior of a compound. It can be divided into two parts, real and imaginary:

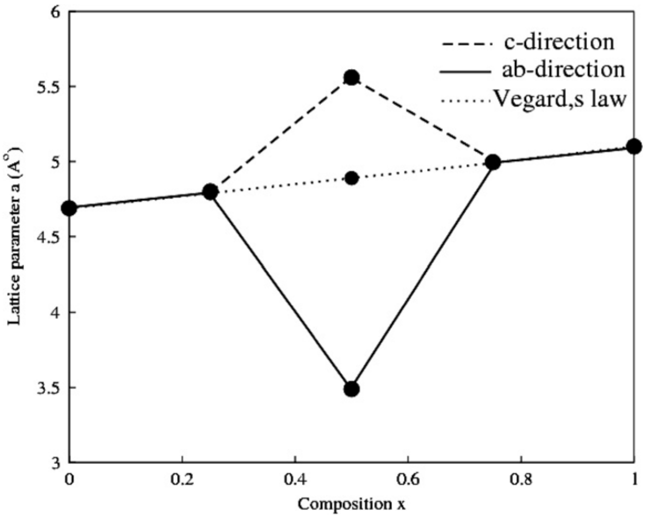

Fig. 2. Variation in lattice constants (*a* and *c*) as a function of composition *x*.

$$\varepsilon(\omega)=\varepsilon_1(\omega)+i\varepsilon_2(\omega) \qquad (3)$$

The imaginary part of the complex dielectric function, $\varepsilon_2(\omega)$, in cubic symmetry compounds can be calculated by the following relation [18,19]:

$$\varepsilon_2(\omega)=\frac{8}{2\pi\omega^2}\sum_{nn'}\int |pnn'(k)|^2\frac{dSk}{\nabla\omega nn'(k)} \qquad (4)$$

while $\varepsilon_2(\omega)$ is used to calculate the real part of the complex