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First principles study of structural, optical, and electronic properties of zinc mercury chalcogenides

G. Murtaza [a,*], Naeem Ullah [b], Abdur Rauf [c], R. Khenata [d], S. Bin Omran [e], M. Sajjad [c], A. Waheed [a]

[a] Materials Modeling Lab, Department of Physics, Islamia College University, Peshawar, Pakistan
[b] Department of Physics, G.D.C. Darra Adam Khel, F.R. Kohat, KPK, Pakistan
[c] Department of Physics, Kohat University, KPK, Pakistan
[d] LPQ3M Laboratory, Faculty of Science and Technology, University of Mascara, Algeria
[e] Department of Physics and Astronomy, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia

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ABSTRACT

First-principles calculations using the full potential linearized augmented plane wave method within the framework of density functional theory are performed to investigate the compositional dependence of the structural, electronic and optical properties of $Zn_{1-x}Hg_xE$ (E=S, Se, Te). It is observed that except the lattice constant, the variation of the bulk modulus and the band gap versus mercury composition does not obey Vegard's law. The alloys at all concentrations have direct band gap ($\Gamma-\Gamma$) which decreases with increasing the concentration of Hg. Optical properties like complex dielectric function and reflectivity are discussed comprehensively. The properties of these materials such as the direct band gap and high absorption in the infrared to ultraviolet regions demonstrate the significant optical activity of these materials.

1. Introduction

The increasing needs of technology enhanced semiconductor processing for optoelectronic devices operating in the visible and far-infrared regions, including light-emitting diodes (LEDs), photo-detectors and solar cells [1–3]. The II–VI semiconductor family contains various wide band gap semiconductors and narrow band gap mercury chalcogenides semiconductors and semimetals exhibiting a large spectrum of properties and making them chief candidates for modern optoelectronic applications [4,5].

A solid solution of two or more semiconductors forms a semiconductor alloy, which has significant technological applications, particularly in the fabrication of electronic and optoelectronic devices [6]. Ternary alloy solid solutions of II–VI semiconductors have been studied in numerous investigations [7–13]. The gas-source molecular beam epitaxy technique has been used by Hara et al. [7] to control the light emission in the visible range while increasing the Hg contents in Zn_{1-x} Hg_xSe. Ternary $Zn_{1-x}Hg_xSe$ and quaternary $Zn_{1-x}Hg_xS_ySe_{1-y}$ alloy layers have been grown on GaAs substrates using molecular beam epitaxy (MBE) and characterized using optical techniques [8]. Electrodepositing studies on $Zn_{1-x}Hg_xSe$ and $Zn_{1-x}Hg_xTe$ have been performed to explore their structural, electronic and optical properties [9,10]. Mahalingam et al. [11] prepared thin alloy films of $Cd_{1-x}Hg_xTe$, $Mn_xHg_{1-x}Te$, and $Zn_xHg_{1-x}Te$ and studied the effect of biaxial stresses in these compounds. Deibuk et al. [12] further used experimental data and mathematical models to study the band gap and optical properties of quaternary

* Corresponding author. Tel.: +92 321 6582416.
E-mail addresses: murtaza@icp.edu.pk (G. Murtaza), khenata_rabah@yahoo.fr (R. Khenata).

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$Cd_xHg_{1-x-y}Zn_yTe$ alloy epitaxial layers. A complete solid solution was obtained throughout the entire range for the ZnHgS system [13].

Because of the importance of zinc and mercury chalcogenides in the modern optoelectronic devices industry, the present work intended to explore the structural, electronic and optical properties of $Zn_{1-x}Hg_xE$ (E=S, Se, Te) in the zinc blende (B3) structure. The modified Becke–Johnson (mBJ) [14] potential approximation was used to overcome the anomaly between the experimental and theoretical when common LDA and GGA approximations [15] are used. The adaptation of mBJ improves the band gap value and the optical spectra that are found in variety of investigations [15,16–18] and the references therein. The mBJ predicts better energy band gaps because it is able to accurately reproduce the exchange potential. It is used for the highly correlated systems with f and d orbitals.

The calculations were performed in the framework of density functional theory (DFT) to treat the electronic band gap, contribution from the different energy levels, optical dielectric constants and refractive indices as a function of composition and energy. Section 2 covers the computational details, Section 3 is devoted to the results and their discussion and in Section 4, the main conclusions are summarized.

2. Computational details

In this work, the calculations were performed employing the full-potential linearized augmented plane wave (FP-LAPW) method as implemented in the Wien2K code [19]. The exchange and correlation effects were treated using the mBJ approximation [14]. Inside the non-overlapping spherical region of the Muffin–Tin radius (R_{MT}) around each atom, a linear combination of the radial solution of the Schrödinger wave equation times the spherical harmonics is used, and in interstitial region, a plane wave basis set was used. The wave function expansion inside the sphere was confined to $l_{max}=10$, while for the expansion of the wave function in the interstitial region, the plane wave cut-off $K_{max}=8/R_{MT}$ was used. Here, K_{max} provides the magnitude of the largest K vector in the plane wave expansion. The integrals over the Brillouin zone are performed up to 1000 k-points in the full Brillouin zone.

Table 1
Atomic positions for $Zn_{1-x}Hg_xTe$ alloys.

x	Atom	Positions
0.25	**Zn**	(0, 0.5, 0.5), (0.5, 0, 0.5), (0.5, 0.5, 0)
	Hg	(0, 0, 0)
	Te	(0.25, 0.75, 0.75), (0.75, 0.25, 0.75), (0.75, 0.75, 0.25), (0.25, 0.25, 0.25)
0.50	**Zn**	(0, 0, 0), (0.5, 0.5, 0)
	Hg	(0.5, 0, 0.5), (0, 0.5, 0.5)
	Te	(0.25, 0.25, 0.25), (0.75, 0.75, 0.25), (0.75, 0.25, 0.75), (0.25, 0.75, 0.75)
0.75	**Zn**	(0, 0, 0)
	Hg	(0.5, 0.5, 0), (0, 0.5, 0.5), (0.5, 0, 0.5)
	Te	(0.25, 0.25, 0.25), (0.75, 0.75, 0.25), (0.75, 0.25, 0.75), (0.25, 0.75, 0.75)

3. Results and discussions

3.1. Structural properties

The structural properties of the binary compounds (ZnS, ZnSe, ZnTe, HgS, HgSe and HgTe) were examined in the zinc blende structure using the generalized gradient approximation of Wu and Cohen (WC-GGA) [20]. Ternary

Table 2
Present calculated equilibrium lattice constant and bulk modulus for $Zn_{1-x}Hg_xE$ along with experimental data and other calculations.

x	a_0 (Å)			B_0 (GPa)		
	Present	**Exp.**	**Others**	**Present**	**Exp.**	**Others**
$Zn_{1-x}Hg_xS$						
0	5.38	5.41[a]	5.30[b], 5.34[c]	81.10	76.90[a]	77.30[d]
0.25	5.545			71.37		
0.50	5.67			68.56		
0.75	5.79			65.68		
1	5.90	5.85[a]	5.97[d]	60.67	68.60[a]	55.30[d]
$Zn_{1-x}Hg_xSe$						
0	5.65	5.67[a]	5.59[a], 5.69[c]	75.68	62.50[a]	83.8[d]
0.25	5.80			62.12		
0.50	5.94			57.41		
0.75	6.05			58.09		
1	6.14	6.07[a]	6.19[b], 6.10[c]	56.36	57.50[a]	41.80[d]
$Zn_{1-x}Hg_xTe$						
0	6.10	6.09[a]	6.02[b], 6.04[c]	56.11	50.09[a]	49.20[d], 52.1[b]
0.25	6.22			52.55		
0.50	6.33			46.25		
0.75	6.43			46.74		
1	6.55	6.46[a]	5.53[b]	43.80	47.60[a]	47.10[d], 46.10[b]

[a] Ref. [27].
[b] Ref. [28].
[c] Ref. [29].
[d] Ref. [30].

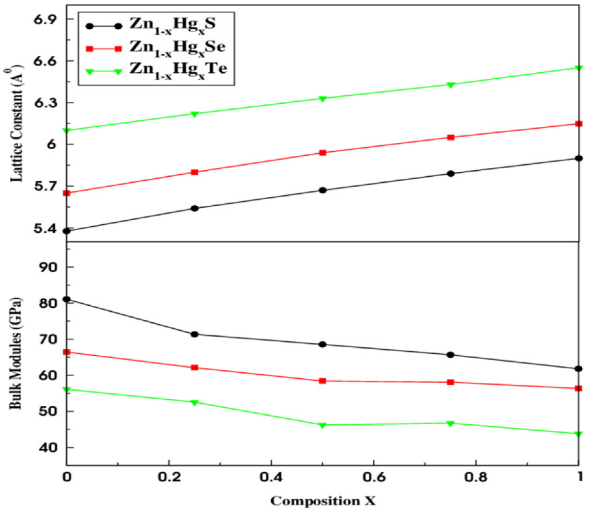

Fig. 1. Composition dependence of calculated lattice constant and bulk moduli of $Zn_{1-x}Hg_xE$ alloys.