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Tailoring Optoelectronic Characteristics of $Zn_xCd_{1-x}S$ Alloys through Band Gap Modulation

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Abstract: In this research, we examine the optical and dielectric characteristics of ZnxCd1-xS, a ternary alloy system with a zinc-blende crystal structure. Our analysis employs a pseudopotential model based on the virtual crystal approximation, which accounts for the effects of compositional disorder. Through our calculations, we investigate various aspects of the refractive index and determine the most suitable model. Additionally, we determine the high-frequency and static dielectric constants for the materials studied. Crucially, we explore the band gap energy of ZnxCd1-xS, which is a fundamental parameter influencing its optical and electronic properties. The ability to tune the band gap energy through compositional variation makes this alloy system particularly attractive for diverse optoelectronic applications, including solar cells, light-emitting diodes, and photodetectors. Our findings show good agreement with previously published results in the literature. These results provide valuable insights for the application of this data in optoelectronics and offer useful information for further research in this field, particularly in the context of band gap engineering for specific device requirements.

1. INTRODUCTION

Semiconductors II–VI are widely used in electronics and optoelectronic devices. These materials have a direct band-gap [1–3] and crystallize in wurtzite or zinc-blende structures and are regarded as excellent candidates for UV and blue applications [4–7]. ZnS and CdS are II-VI semiconductor compounds with wide band gaps that crystallize in wurtzite or zinc-blende [8, 9]. One method for practically continuously changing the energy band gap of semiconducting materials over a wide variety of energies is to use ternary alloys [10–13]. $Zn_xCd_{1-x}S$ can be made by combining CdS and ZnS, given the importance of $Zn_xCd_{1-x}S$ in technological applications. This work estimates the optical characteristics and energy band structure of $Zn_xCd_{1-x}S$ using a revised VCA that involves the disorder of the alloy. The purpose of this

investigation is to determine how much the disorder impact affects the optical characteristics and band structure energies of $Zn_xCd_{1-x}S$.

2. COMPUTATIONAL METHOD

The (EPM) technique is utilized to compute the energy band structure [14–16], while the alloy's potential is calculated using the improved virtual crystal approximation as shown in [17, 18],

$$V_{alloy}(r) = V_{VCA}(r) + V_{dis}(r) \tag{1}$$

The disorder effect provides a non-periodic potential, namely $V_{dis}(r)$ in equation (1). The equation used to calculate the pseudopotential form factors is written as follows:

$$V_{alloy}(G) = (1-x)V_{CdS}(G) + xV_{ZnS}(G) - p\left[x(1-x)\right]^{\frac{1}{2}}\left(V_{ZnS}(G) - V_{CdS}(G)\right) \tag{2}$$

In this case, G is a reciprocal lattice vector, and p is a factor that can be changed. When the compositional disorder is considered, the value of p is -0.045, resulting in a band gap bowing value of roughly 0.83 eV. This number is similar to the 0.827 eV found by [19, 20]. The method of a non-linear least-squares is used to change the defined form factors. [21-23]. The band-gap energies chosen in the fitting for ZnS and CdS are shown in Table 1. The resulting adjusted form factors and lattice parameters for ZnS and CdS are shown in Table 2.

Table 1. Band gap energies fixed in the fits for ZnS and CdS.

Compound	**$E_{\Gamma-\Gamma}$ (eV)**	**$E_{\Gamma-X}$ (eV)**	**$E_{\Gamma-L}$ (eV)**
CdS	2.36 [a]	3.64 [a]	3.50 [a]
ZnS	3.9 [b]	3.8 [c]	4.90 [d]

[a] [24]; [b] [25]; [c] [26]; [d] [27].

Table 2. Pseudopotential parameters for ZnS and CdS.

Compound	**Form factors (Ry)**						Lattice constant (Å)
	$V_S(3)$		$V_S(11)$	$V_A(3)$	$V_A(4)$	$V_A(11)$	
CdS	-0.23	5.83	0.06	0.134	0.096	0.019	5.83
ZnS	-0.396388	6.48	0.459548	0.1311	0.28	0.708145	6.48

As shown below, the refractive index (n) was calculated using three distinct models, all of which are directly related to the energy band-gap.

(i). Based on an atomic model, the Moss formula [28] is:

$$E_g n^4 = k \tag{3}$$

Where E_g represents the energy band gap and k=108 eV [28].

(ii). The Ravindra et al. [29] relation, (4)

Here $\alpha = 4.084$ and $\beta = -0.62\, eV^{-1}$

(iii). The Hervé and Vandamme [30] empirical equation ,

$$n = \sqrt{1 + \left(\frac{A}{E_g + B} \right)^2} \tag{5}$$

With $A = 13.6\, eV$ and $B = 3.4\, eV$

3. RESULTS AND DISCUSSION

The calculated electronic band structure of zinc-blende $Zn_{0.50}Cd_{0.50}S$ is shown in Figure 1, with consider or not the compositional disorder. The maximum of the valence bands is at Γ. The minimum of conduction band can also be found at Γ. As a result, $Zn_{0.50}Cd_{0.50}S$ is a direct band-gap. It should be noted that the The distribution of the valence bands is substantially lower, the condition bands are more delocalized. In terms of quality, the general shapes of both are remarkably similar to the binary compound. It should be underlined that compositional disorder is irrelevant on the electronic structure of $Zn_{0.50}Cd_{0.50}S$. The composition dependency of the

refractive index determined using the (3-5) relationships is shown in Figure 2 (a) and (b) with and not consider the effect of disorder. It should be observed that the change in n versus x for all models evaluated, has a non-linear tendency. The principal consequences of disorder are assumed to be responsible for this non-linearity. The models used show the same monotonic declining trend qualitatively. For various compositions x, the high-frequency dielectric constant has been approximated utulizing the equation:

$$\varepsilon_{\infty} = n^2 \tag{6}$$

Figure 3 illustrates our findings, the declines in ε_{∞} with rising x during the change from CdS to ZnS, demonstrating a definite non-linear tendency for all models examined. When the high-frequency dielectric constants decrease with increasing composition x, the material's polarity and capacity decrease to stabilize charges.

4. CONCLUSION

Finally, the energy band structure and optical characteristics of $Zn_xCd_{1-x}S$, ternary semiconductor alloys have been examined in terms of composition x. Our results are founded on the EPM, using a revised VCA that consider the effet of compositional disorder. This had no effect on the energy band structure of $Zn_xCd_{1-x}S$, and it was found that this semiconductor had a direct-band gap across the full Zn concentrations x in the range ($0 \leq x \leq 1$). Our findings are fairly consistent with the available experimental and theoretical data reported in the literature. In all models studied, the refractive index and high-frequency dielectric constant ε_{∞} altered nonlinearly with regard to x, indicating that alloy disorder caused a slight but considerable bowing parameter.

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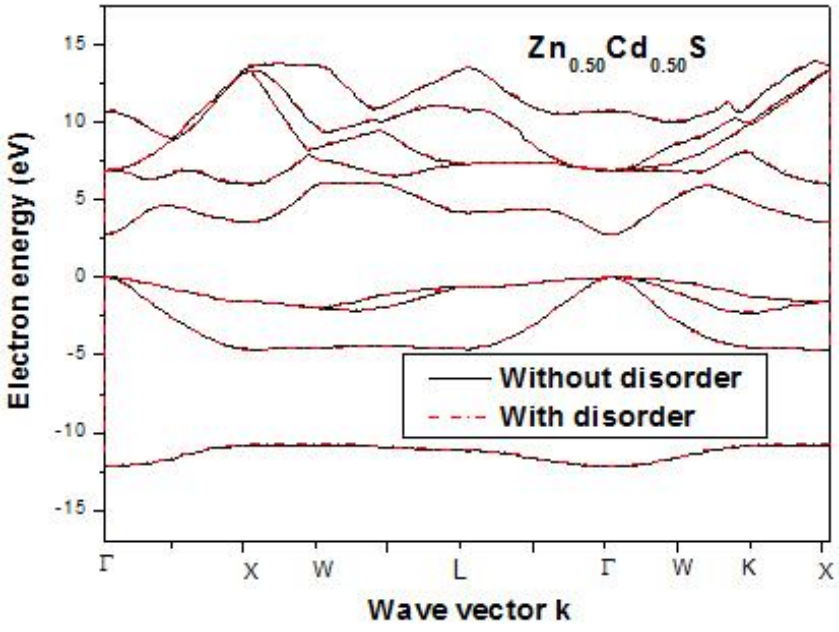

Fig.1. Electronic band structure of zinc-blende $Zn_{0.50}Cd_{0.50}S$.

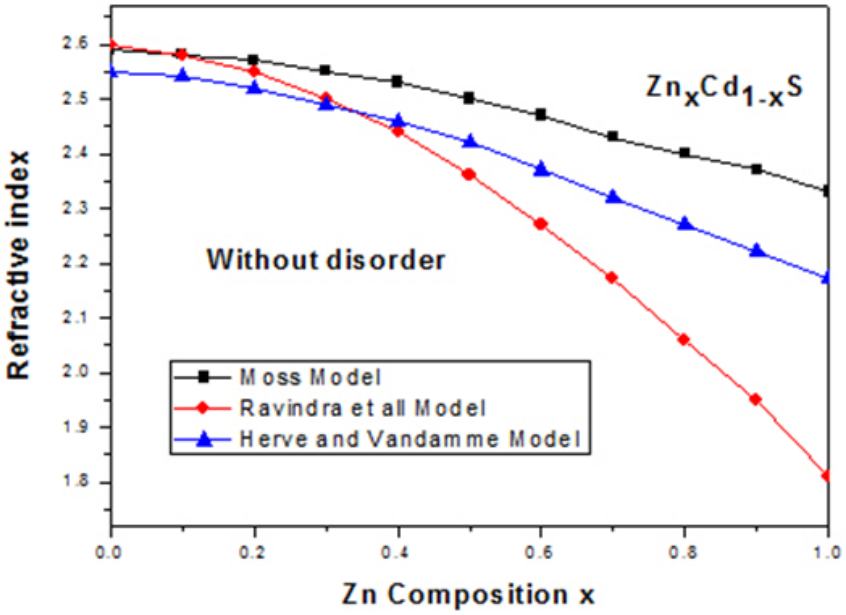

Fig.2 (a). Refractive index as a function of Zn composition x, in $Zn_xCd_{1-x}S$ without disorder

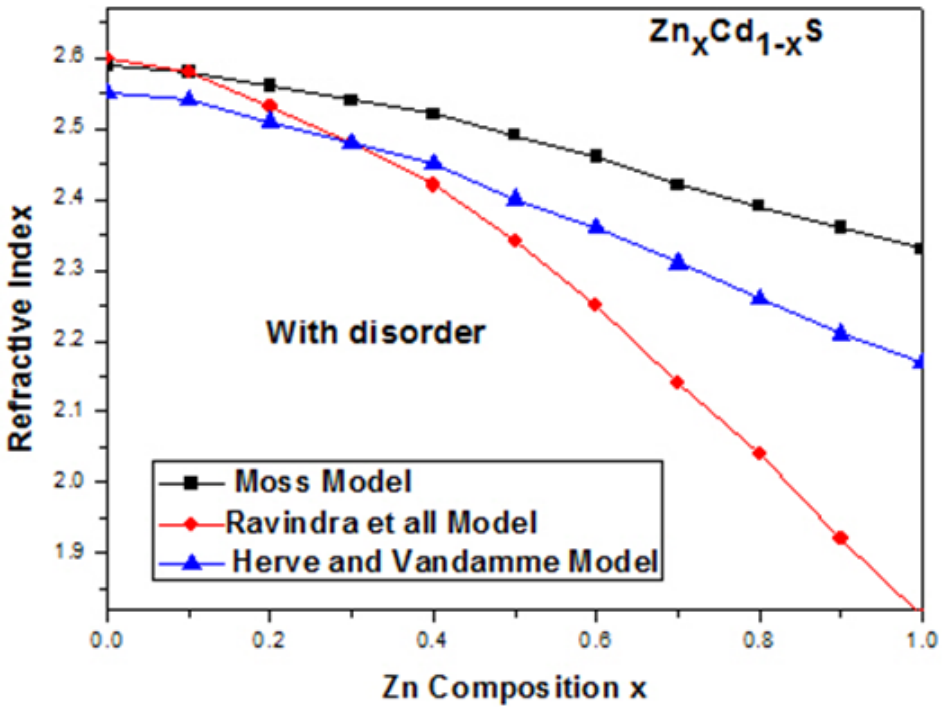

Fig.2 (b). Refractive index as a function of Zn composition x, in $Zn_xCd_{1-x}S$ with disorder

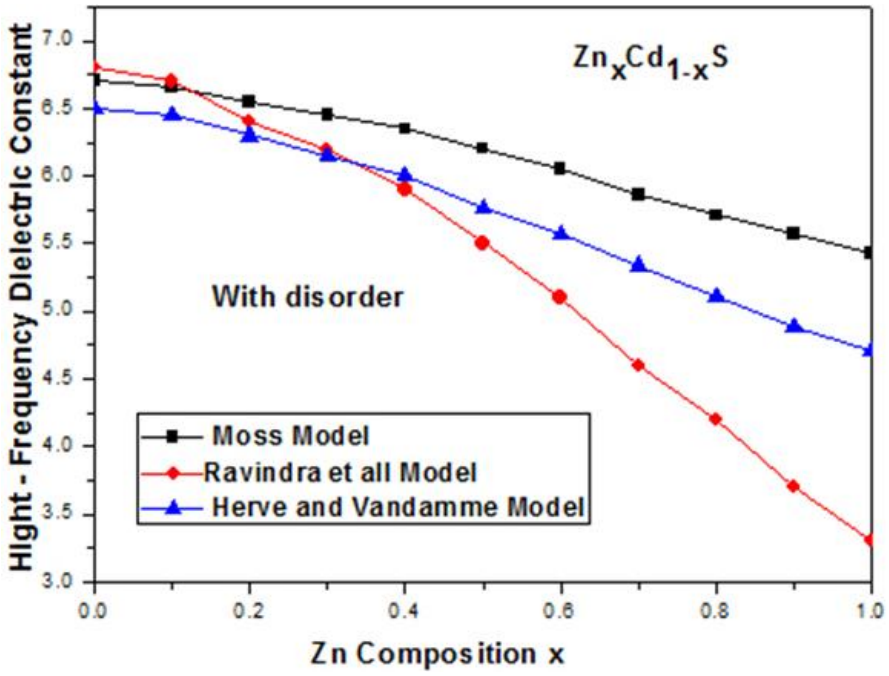

Fig.3. High-frequency dielectric constant function of Zn composition x, in $Zn_xCd_{1-x}S$ with disorder