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Contents

Functional Materials
1  Heteromorphic Hematite Pigments Obtained from Steel Scrap and Encapsulated in Amorphous Silica for Porcelainized Stoneware
   Viviana Possamai Della, Janaina Accordi Junkes, Antonio Pedro Novaes de Oliveira and Dachamir Hotza
14  Constitutive Model for Glassy-Active Phase Transformation on Shape Memory Polymers Considering Small Deformations
   Manuel Ignacio Varela-Jimenez, Jorge A. Cortes-Ramirez and Yi-chao Chen
23  Synthesis, Characterization and Antimicrobial Activity of Nano ZnO and Pd Loaded Nano ZnO against Enteric Pathogens
   Muhammad Akram Randhawa, Alhusain Jaber Al-Zahrani, Muhammad Ashraf Gondal and Abdul Aziz Bagabas
27  Compliance Experimental Determination in Nonstandard SEN Samples in API 5L Steel Pipe in the Short Radial Direction
   Daniel Angeles Herrera, González Velázquez Jorge Luis and Morales Ramírez Ángel de Jesús

Structural Materials
33  NiO-CGO Composite for SOFC Anode: Synthesis and Characterization
   Beatriz Cela, Daniel Araújo de Macedo, Graziele Lopes de Souza, Auristela Carla de Miranda, Antonio Eduardo Martinelli, Rubens Maribondo do Nascimento and Carlos Alberto Paskocimas
40  Effect of Ettringite Crystallization Inhibitors on Expansion Rate of Expansion Admixture
   Zhongcheng Ma, Lan Wang and Guojin Ji
46  Influence of the Solidification on the Microstructure and Microhardness of Undercooled Al_{96}Fe_{2}Nd_{2} Alloy
   Walman Benicio de Castro and Benedito Antonio Luciano
51  Effect of Temperature on Titanium Dioxide in Polyethylene Terephthalate Protective Coatings on ECCS Steels
   Ernesto Zumelzu, Claudio Ortega and Fernando Rull
57  Effect of Heat Treatment on Microstructure of Cu-Al Alloys under 1GPa
   Jinquan Lu, Chunyan Deng, Tao Xu, Guirong Peng, Jianhua Liu and Ruijun Zhang
61  Study by Fourier Transform Infrared Spectroscopy of the Avocado Oils Varieties Hass, Criollo and Fuerte
   José Alberto Ariza-Ortega, María Guadalupe Méndez-Ramos, Joel Diaz-Reyes, Raúl Jacobo Delgado-Macuil and Raúl René Robles-de-la-Torre
65  Fabrication and Characterization of Crack Free Nano Porous Titanium Dioxide Thin Films by Spray Deposition Technique
   Manzar Abbas, Nazar Abbas Shah, Fazali Subhan and Muhammad Irfan

Theoretical Researches
71  Vibration on Building: A Stability Analysis Using PID Controller
   Mohd Azli Salim, Mohd Khairi Mohamed Nor and Aminurrashid Noordin
80  Quantum Dot Potential Calculation of Zn_{x}Cd_{1-x}Se
   Yarub Al-Douri, Naser M. Ahmed and Uda Hashim
Quantum Dot Potential Calculation of Zn$_x$Cd$_{1-x}$Se

Yarub Al-Douri, Naser M. Ahmed and Uda Hashim

Institute of Nano Electronic Engineering (INEE), University Malaysia Perlis (UniMAP), Kangar, Perlis 01000, Malaysia

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Abstract: The indirect energy gaps ($\Gamma$-$X$) are calculated using Empirical Pseudopotential Method (EPM) for ZnSe and CdSe semiconductors. The obtained band gaps of semiconductors that form the Quantum Dot (QD) of Single Electron Transistor (SET) are used to calculate the quantum dot potential within our recent model. Also, the energy gap of $\Gamma$, $X$ and $L$ and the quantum dot potential as a function of alloy concentration are studied for Zn$_x$Cd$_{1-x}$Se alloys. For the ternary alloy Zn$_x$Cd$_{1-x}$Se, the virtual crystal approximation (VCA) is coupled with the pseudopotential method. Band structure of Zn$_{0.5}$Cd$_{0.5}$Se is also calculated.

Key words: Zn$_x$Cd$_{1-x}$Se, Quantum Dot, EPM.

1. Introduction

Wide band gap II-VI heteroepitaxy has attracted considerable attention in the last two decades due to potential applications in blue-light emission diodes and lasers. However, the fundamental aspect of p-type doping is still in severe challenge because of strong self-compensation in II–VI wide band gap semiconductors. The recent development of II-VI CdS/ZnSe [1], (CdS/ZnSe)/BeTe [2] and ZnCdSe/ZnCdMgSe [3] quantum wells (QWs) has opened up application in mid- and near-infrared (IR) region using the intersubband (ISB) transitions within the conduction band of the QW, i.e., unipolar devices such as IR photodetectors, quantum cascade lasers (QCL), as well as ultrafast all-optical switches (UOS). Previously, it has been proposed that the II-VI-based QWs are the promising candidates for UOS at near-IR wavelength region due to the enhanced electron–phonon interaction [2]. Bulk Zn$_x$Cd$_{1-x}$Se crystallizes either in the cubic zinc blende structure ($x>0.7$), in the hexagonal wurtzite structure ($x<0.5$) or in mixture of these two for $0.5 \leq x \leq 0.7$ [4]. However, growing Zn$_x$Cd$_{1-x}$Se on GaAs (1 0 0) substrate with molecular beam epitaxy (MBE) results in films of zinc blende structure over the entire range of composition.

Literature values for the energy gap of zinc blende CdSe at 300 K vary from 1.66 to 1.74 eV. Spectroscopic elipsometric measurements are found in a value of 1.74 eV [5, 6] as well as a value of 1.66 eV [7]. Reflection spectroscopic [8] and photomodulation spectroscopy [9] yield a value of 1.66 eV at 300 K. The energy gap of Zn$_x$Cd$_{1-x}$Se alloy has been determined at 300 K by reflection spectroscopy [10] and spectroscopic ellipsometry [7]. To further enhance our understanding of quantum dot potential (QDP) of Zn$_x$Cd$_{1-x}$Se ternary material for device application, an empirical pseudopotential band structure calculation for this alloy has been carried out. In this paper, the calculated results of band gap for various compositions are presented. The empirical pseudopotential method [11] (EPM) has been proven to be one of the most reliable methods for band structure calculation of semiconductors and high techniques parameters study. In comparison, the self consistent pseudopotential method in the local density approximation (LDA) usually underestimates the energy band [12]. In the empirical pseudopotential method, the actual atomic potential is replaced by pseudopotential and a set of atomic form factors where adjusted, so that the...
calculation produces energy bands as accurately as possible in the whole composition range with existing experimental data. Together with the virtual crystal approximation (VCA) the EPM offers the most effective and accurate means of obtaining the band structure of alloy. In the following title, the pseudopotential method applied to semiconductor alloy is presented. Electronic band structure and QDP results of our VCA calculations for Zn$_x$Cd$_{1-x}$Se ordered alloy are displayed in the later.

2. Calculation Method

Let us define the empirical pseudopotential (EPP) of a semiconductor as a superposition of pseudatomic potentials of the form $V = V_L + V_{NL}$, where $V_L$ and $V_{NL}$ are local and non-local parts, respectively. In this calculation, the non-local part is omitted. In the EPP composed of a small number of parameters consistent with electronic energy band structure (EBS) over a wide range, these parameters should be determined to be fully interdependent among them. Since, with the availability of the experimental data, some of authors [13] attempted to understand the EBS of semiconductors in a wide energy range.

The pseudopotential Hamiltonian:

$$H = -\frac{n}{2m} \nabla^2 + V_i(\mathbf{r}),$$  \hspace{1cm} (1)

contains an effective potential, which is expanded as Fourier series in a reciprocal space. For binary compounds the expression is written in two parts, which are symmetric and antisymmetric with respect to interchange of the two atoms about their mid-point:

$$V_i(\mathbf{r}) = \sum_q \left[ S_q^a(G) V^a(G) - i S_q^b(G) V^b(G) \right] \exp(i\mathbf{G}\cdot\mathbf{r}), \hspace{1cm} (2)$$

where $S(G)$ and $V(G)$ are structure and form factors. The EPP by the nonlinear least square method are determined, in which all the parameters are determined automatically in an independent way. The lattice constant of the alloy $K = K_i$ in the plane wave representation and $i$th pseudo wave function at $K = K_i$ is expanded as:

$$\psi_{K_i}(\mathbf{r}) = \sum_q C_q^{i}(K_i) \exp[i(K_i + G_q)\mathbf{r}], \hspace{1cm} (7)$$

where $G_q$ is the reciprocal lattice vector. Eq. (7) shows that all the parameters are determined automatically in an independent way. The lattice constant of the alloy AB$_{1-x}$C$_x$ (AC: ZnSe, BC: CdSe) is assumed to follow Vegard’s law:

$$a(x) = (1-x) a_{AC} + x a_{BC}, \hspace{1cm} (8)$$

where $x$ is the mole fraction, and $a_{AC}$ and $a_{BC}$ are the lattice constants of the pure semiconductors AC and BC, respectively. Note that as the lattice constant is function of the alloy concentration $x$, the reciprocal vectors are also dependent upon $x$.

3. Results and Discussion
3.1 Electronic Band Structure

The pseudopotential form factors for the pure components ZnSe and CdSe are shown in Table 1. They give the reasonable agreement with experiment and other calculations for the principal energy gaps (Table 2). With the VCA the curves for the conduction \( \Gamma, X \) and \( L \) valleys of this alloy versus concentration of Zn are given in Fig. 1. The reference energy level is the top of the valence band. It is clear that Zn\(_x\)Cd\(_{1-x}\)Se is a semiconductor and the calculated variation of the energy gap was found to be linear with mole fraction as shown in Fig. 1.

In Fig. 2, one can show the calculated band structure of Zn\(_{0.5}\)Cd\(_{0.5}\)Se. The band structure is typical of the zinc blende material. The alloy exhibits a direct gap for the given composition. The horizontal axis corresponds to energy, referenced by \( E_v \). The cubic ternary alloy of Zn\(_{0.5}\)Cd\(_{0.5}\)Se has valence band qualitatively similar to ZnSe [13, 17]. The second state of the second valence band is primarily of cation s character, it changes rapidly to anion p-like at the top of the valence band. The conduction bands are more difficult to describe than the valence bands because they are more delocalised and more “free-electron-like” than the valence states. This is particularly true for the conduction band states far removed from the VBM. The free-electron behaviour results in more dispersive bands.

3.2 Quantum Dot Potential

The II-VI semiconductors such as ZnSe and CdSe are among the most ionic solids, which crystallise in zinc blende structure. The ionic contribution to the bonding is very large compared to \( \text{sp}^3 \) bonding. This can also express in terms of potential calculation of high technique of quantum dot using our recent model [18].

### Table 1
<table>
<thead>
<tr>
<th></th>
<th>( V_s(3) )</th>
<th>( V_s(8) )</th>
<th>( V_s(11) )</th>
<th>( V_a(3) )</th>
<th>( V_a(4) )</th>
<th>( V_a(11) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>CdSe</td>
<td>11.4324</td>
<td>-0.23</td>
<td>0.01</td>
<td>0.01</td>
<td>0.19</td>
<td>0.12</td>
</tr>
<tr>
<td>ZnSe</td>
<td>10.67851</td>
<td>-0.23194</td>
<td>0.00523</td>
<td>0.06281</td>
<td>0.17773</td>
<td>0.13004</td>
</tr>
</tbody>
</table>

### Table 2

<table>
<thead>
<tr>
<th></th>
<th>( E_{\Gamma \Gamma} )</th>
<th>( E_{\Gamma X} )</th>
<th>( E_{\Gamma L} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>CdSe</td>
<td>Cal. 1.9</td>
<td>Exp.(^a) 1.9</td>
<td>Theor. 2.8</td>
</tr>
<tr>
<td>ZnSe</td>
<td>Cal. 5.4</td>
<td>Exp.(^b) 3.875</td>
<td>Theor. 4.499</td>
</tr>
<tr>
<td></td>
<td>Cal. 4.7</td>
<td>Exp.(^c) 3.612</td>
<td>Theor. 4.499</td>
</tr>
</tbody>
</table>

\(^a\) Ref. [14], \(^b\) Ref. [15], \(^c\) Ref. [16].

Fig. 1 Calculated values of E\( \Gamma \), E\( \Gamma X \), E\( \Gamma L \) gaps for Zn\(_x\)Cd\(_{1-x}\)Se plotted as a function of alloy concentration (VCA calculation).

Fig. 2 Calculated band structure of Zn\(_{0.5}\)Cd\(_{0.5}\)Se.
Quantum Dot Potential Calculation of Zn$_x$Cd$_{1-x}$Se

Fig. 3 Variation of quantum dot potential with alloy concentration for Zn$_x$Cd$_{1-x}$Se.

The calculated results are in reasonable agreement with Udipi et al. [19]. The variation of QDP versus concentration of Zn for Zn$_x$Cd$_{1-x}$Se alloy is displayed in Fig. 3.

The results show linear variation of QDP for this alloy. It indicates that for all Zn concentration, the QDP values do not exceed that of their end-point parents. This result confirms the overall trends observed for the energy levels calculation. Other feature linked to the QDP is the gap at point X. This “antisymmetric” gap has been proposed as a measure of technological properties. As noticed that the trend follows that of the QDP obtained above. This result is very interesting in regard to the structure phase transition of this alloy.

4. Conclusions

Electronic band structure and QDP of Zn$_x$Cd$_{1-x}$Se alloy are calculated using empirical pseudopotential method. It is shown that Zn$_x$Cd$_{1-x}$Se is found to be a semiconductor with a small direct gap. The result of the technological properties confirms the fact that this study is the most appropriate for the II–VI semiconductors. QDP is calculated. A good agreement with experimental and theoretical data was observed.

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References


