CODEN: IAASCA   **ORIGINAL ARTICLE**

Refractive Index and Dielectric constant of Barium Chalcogennide Ternary alloys

P.K.Singh[a]*, Sanjay Singh[b], Sharad Yadav [c]and S.B. Sharma[d]
[a]Department of Physics, Shri Sadguru Saibaba Science College, Ashti, Gadchiroli, Maharastra, India
[b]Department of Physics, Chintamani Science & Arts College, Gondpipari, Chandrapur, Maharastra, India
[c] Department of Physics, IBS, Dr. Bhimrao Ambedkar University, Khandari Campus, Agra
[d]DDIVE, Dr. Bhimrao Ambedkar University, Khandari Campus, Agra

ABSTRACT

We have used four different models due to Moss, Ravendra et al, Vandamme, and Full Potential Linearized Augmented Plane Wave (FP-LAPW) due to Drablia et al for determining refractive index and dielectric constant for barium chalcogenide ternary alloys. The results have been obtained for the entire range of compositions in case of $BaS_{1-x}O_x$, $BaS_{1-x}Se_x$ and $BaS_{1-x}Te_x$. It is found that the results based on different empirical models are in close agreement with each other but significant derivation have been found for the results based on the FP-LAPW. The comparison of results reveals that a correction term is needed for the theoretical model based on the FP-LAPW method.
Keywords: Potential linearized augmented plane wave method, Optoelectronic properties, Chalcogenides, Alloys.
PACS: 61.66.Dk, 71.15.Mb, 71.15.Nc, 71.20.Nr, 78.20.Ci

INTRODUCTION

The optoelectronic properties of alkaline earth chalcogenides (AEC) have been studied in terms of refractive index and optical or electronic dielectric constant. In the models based on the first principles calculations, we use the energy gap formulations [1]. Using the Potential Linearized Augmented Plane Wave (FP-LAPW) method [2] and empirical relations due to Moss[3], Ravindra et al [4] and Vandamme's formula [5] the refractive index and the optical dielectric constant have been calculated as a function of composition x. The results for all the methods used show that the refractive index as well as optical dielectric constant change non-linearly with respect to composition x exhibiting different bowing parameters which arise from the effects of compositional alloy disorder. The results obtained from FP-LAPW method for the parent compounds show better agreement with the available experimental data. A significant deviation of the lattice constant from Vegard's law has been observed for $BaS_{1-x}O_x$ alloy, while the calculated lattice parameters at different compositions for $BaS_{1-x}Se_x$ and $BaS_{1-x}Te_x$ alloys were found to vary almost linearly.

Barium chalcogenide compounds (BaX, X=O, Se and Te) have attracted increasing interest due to their potential applications in light-emitting diodes (LEDs) and laser diodes (LDs). They are technologically important materials with many applications ranging from catalysts to microelectronics and in the area of luminescent and magneto-optical devices [6-9]. The optoelectronic properties of semiconductors alloy are essential in the design and analysis of devices mentioned above, the electronic energy levels, the refractive indices and the optical dielectric constants of the material of interest have to be known as a function of composition and wavelength.

The experimental [10] and theoretical [11-14] studies of BaX (X=O, S, Se and Te) compounds have been made by many researchers. Most of available experimental results on the reflectivity and absorption of these compounds are limited to excitonic transitions [15]. From a theoretical point of view, the electronic properties of BaS, BaSe and BaTe have been determined by Pourghazi and Dadsetani [16] using full FP-LAPW method. The elastic and bonding properties of BaS, and BaTe have been calculated by Hassan and Akbarzadeh [13]. BaO compound has been studied by Habas et al. [17]. Using the available data on various parameters we proceed to obtain results for refractive index and dielectric constant.

METHOD OF ANALYSIS

Optical properties of a solid are usually described in terms of the complex dielectric function

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \qquad (1)$$

The imaginary part of the dielectric function in the long wavelength limit has been obtained directly from the electronic structure calculation, using the joint density of states and the optical matrix element. The real part of the dielectric function can be derived from the imaginary part by the Kramers-Kroning relation. The knowledge of both the real and the imaginary parts of the dielectric function allows the calculation of important optical functions. The refractive index $n(\omega)$, is given by:

$$n(\omega) = \left[\frac{\varepsilon_{1(\,)}\,\omega}{2} + \frac{\sqrt{\varepsilon_{,}^{2}\,(\omega) + \varepsilon_{2}\,(\omega)}}{2} \right]^{1/2} \tag{2}$$

At low frequency ($\omega = 0$), we get the following relation:

$$n(0) = \left[\varepsilon(o) \right]^{1/2} \tag{3}$$

The refractive index and optical dielectric constant are very important to determine the optical and electrical properties of the crystal. Advanced applications of compounds can significantly benefit from accurate index data. The use of fast non-destructive optical techniques for epitaxial layer characterization (determination of thickness or alloy composition) is limited by the accuracy with which refractive indices can be related to alloy composition. These applications require an analytical expression of known accuracy to relate the wavelength dependence of refractive index to alloys composition, as determined from simple techniques as photoluminescence. A few empirical relations [3-5] relate the refractive index to the energy band gap for a large set of semiconductors. However, in these relations the refractive index n is independent of the temperature and the incident-photon energy. The following models are used:

The Moss formula [3] based on atomic model:

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

where E_g is the energy band gap and k is a constant with a value of 108 eV [3].
The Ravindra et al. [4] relation,

$$n = \alpha + \beta\, E_g \tag{5}$$

with $\alpha = 4.084$ and $\beta = -0.62 \text{eV}^{-1}$,
Vandamme's empirical relation [5]:

$$n = \sqrt{ 1 + \left(\frac{A}{E_g + B} \right)^2 } \tag{6}$$

with A=13.6 eV and B=3.4eV.

RESULTS AND DISCUSSIONS
Equations (4)-(6) are useful for determine the refractive index n of pure crystals as well as can be applied for mixed crystal or alloys. The composition dependence of the refractive index has been calculated according to the FP-LAPW method and equations (4)-(6). The refractive index increases or decreases monotonically with increasing of Se or Te content through the entire range of composition x=0 to x=1 for

the $BaS_{1-\chi}Se_{\chi}$ and $BaS_{1-\chi}Te_{\chi}$ alloys. For the $BaS_{1-\chi}O_{\chi}$ alloy, the variations are not monotonous. The calculated refractive indices versus concentration were fitted by a polynomial equation[18]. The results are summarized in Tables 1-6. Here $n_1(x)$, $n_2(x)$, $n_3(x)$ and $n_4(x)$ are referred to as the refractive index obtained from FP-LAPW method and the empirical models based on equations (4)-(6) respectively. For

the $BaS_{1-\chi}O_{\chi}$ alloy, important upward bowings are observed for $n_2(x)$, $n_3(x)$ and $n_4(x)$ compared

to $n_1(x)$. However, for BaS$_{1-x}$Se$_x$ marginal upward bowings are obtained when the empirical relations are used. Interestingly, we note on going from BaS to BaSe or BaTe the band gap of the BaS$_{1-x}$Se$_x$ and BaS$_{1-x}$Te$_x$ alloys decreases whereas, the refractive index increases. The ternary alloys show that the smaller band gap material has a large value of the refractive index as the general behaviour of many other groups III-V semiconductors alloys [19].

Table 1: Values of refractive indices as a function of composition x for BaS$_{1-x}$O$_x$ calculated from different formulations.

X	n$_1$	n$_2$	n$_3$	n$_4$
0	2.258	2.676	2.762	2.643
0.1	2.242	2.740	2.873	2.747
0.2	2.224	2.788	2.959	2.824
0.3	2.205	2.822	3.020	2.873
0.4	2.184	2.841	3.054	2.896
0.5	2.162	2.846	3.064	2.890
0.6	2.138	2.835	3.048	2.858
0.7	2.112	2.809	3.006	2.797
0.8	2.085	2.769	2.939	2.710
0.9	2.057	2.713	2.846	2.595
1	2.027	2.643	2.728	2.453

n$_1$ from FP-LAPW model; n$_2$ from Moss relation; n$_3$ Ravindra relation; n$_4$ Vandamme's relation

Table 2: Values of optical dielectric constants as a function of composition x for BaS$_{1-x}$O$_x$ calculated from different formulations.

X	ε$_1$	ε$_2$	ε$_3$	ε$_4$
0	5.102	7.170	7.655	7.004
0.1	5.028	7.519	8.296	7.568
0.2	4.948	7.787	8.790	7.984
0.3	4.862	7.972	9.136	8.252
0.4	4.771	8.076	9.333	8.373
0.5	4.674	8.098	9.383	8.346
0.6	4.571	8.038	9.285	8.171
0.7	4.463	7.896	9.040	7.849
0.8	4.350	7.672	8.646	7.379
0.9	4.230	7.367	8.104	6.761
1	4.105	6.979	7.415	5.995

ε$_1$ from FP-LAPW model; ε$_2$ from Moss relation; ε$_3$ Ravindra relation; ε$_4$ Vandamme's relation

Table 3: Values of refractive indices as a function of composition x for BaS$_{1-x}$Se$_x$ calculated from different formulations.

x	n$_1$	n$_2$	n$_3$	n$_4$
0	2.258	2.637	2.700	2.613
0.1	2.239	2.645	2.717	2.624
0.2	2.226	2.652	2.732	2.634
0.3	2.220	2.660	2.747	2.644
0.4	2.220	2.667	2.761	2.653
0.5	2.225	2.674	2.774	2.662
0.6	2.237	2.680	2.787	2.670
0.7	2.255	2.686	2.798	2.678
0.8	2.279	2.692	2.808	2.686
0.9	2.310	2.698	2.818	2.693
1	2.346	2.703	2.827	2.699

n$_1$ from FP-LAPW model; n$_2$ from Moss relation; n$_3$ Ravindra relation; n$_4$ Vandamme's relation

Table 4: Values of optical dielectric constants as a function of composition x for BaS$_{1-x}$Se$_x$ calculated from different formulations.

x	ε$_1$	ε$_2$	ε$_3$	ε$_4$
0	5.101	6.958	7.292	6.831
0.1	5.015	6.999	7.383	6.888
0.2	4.956	7.039	7.470	6.942
0.3	4.926	7.078	7.553	6.994
0.4	4.924	7.115	7.631	7.043
0.5	4.950	7.150	7.704	7.090

0.6	5.004	7.184	7.773	7.134
0.7	5.085	7.216	7.837	7.176
0.8	5.195	7.247	7.897	7.216
0.9	5.333	7.277	7.953	7.253
1	5.499	7.305	8.004	7.288

ε_1 from FP-LAPW model; ε_2 from Moss relation; ε_3 Ravindra relation; ε_4 Vandamme's relation

Table 5: Values of refractive indices as a function of composition x for $BaS_{1-x}Te_x$ calculated from different formulations.

x	n_1	n_2	n_3	n_4
0	2.259	2.638	2.703	2.614
0.1	2.259	2.672	2.767	2.657
0.2	2.264	2.702	2.824	2.697
0.3	2.274	2.730	2.875	2.732
0.4	2.290	2.754	2.919	2.764
0.5	2.311	2.776	2.958	2.791
0.6	2.337	2.795	2.989	2.814
0.7	2.369	2.810	3.015	2.833
0.8	2.406	2.823	3.034	2.848
0.9	2.448	2.833	3.047	2.859
1	2.496	2.840	3.053	2.866

n_1 from FP-LAPW model; n_2 from Moss relation; n_3 Ravindra relation; n_4 Vandamme's relation

Table 6: Values of optical dielectric constants as a function of composition x for $BaS_{1-x}Te_x$ calculated from different formulations.

x	ε_1	ε_2	ε_3	ε_4
0	5.108	6.960	7.304	6.835
0.1	5.101	7.140	7.662	7.069
0.2	5.120	7.305	7.985	7.281
0.3	5.166	7.455	8.273	7.473
0.4	5.239	7.589	8.528	7.643
0.5	5.338	7.707	8.747	7.792
0.6	5.463	7.810	8.932	7.920
0.7	5.615	7.897	9.082	8.027
0.8	5.793	7.969	9.198	8.112
0.9	5.998	8.026	9.279	8.177
1	6.230	8.067	9.326	8.220

ε_1 from FP-LAPW model; ε_2 from Moss relation; ε_3 Ravindra relation; ε_4 Vandamme's relation

The optical dielectric constant has been estimated according to the expressions given by Drablia et al [1], the results are given in Tables 1-6 It seems that the FP-LAPW method leads to the values for ε deviate significantly from the other empirical models. Qualitatively, the compositional dependence of the dielectric function of the alloys has the same trend as that of the refractive index. This is not surprising as the dielectric function and refractive index both are related to each other. The theoretical method used by Drablia et al [1] needs to be modified in order to make it compatible with the empirical models which have been developed using the experimental values of band gap energies and dielectric constants.

REFERENCES

1. S. Drablia, H. Meradji, S. Chemid, G. Nouet, F.El Haj Hassan, Computational Materials Science 46 (2009) 376.
2. O.K. Anderson, Phys. Rev. B 42 (1975) 3060.
3. V.P. Gupta, N.M. Ravindra, Phys. Stat. Sol. B 10 (1980) 715.
4. N.M. Ravindra, S. Auluck, V.K. Srivastava, Phys. Stat. Sol. B 93 (1979) 155.
5. J.P.L. Herve, L.K.J. Vandamme, Infrared Phys. Technol. 35 (1994) 609.
6. T.A. Grzybowski, A.L. Ruoff, Phys. Rev. B 27 (1983) 6502.
7. T.A. Grzybowski, A.L. Ruoff, Phys. Rev. Lett. 53 (1984) 489.
8. S.T. Weir Y.K. Vohra, A.L. Ruoff, Phys. Rev. B 33 (1986) 4221; S.T. Weir, Y.K. Vohra, A.L. Ruoff, Phys. Rev. B 35 (1987) 874.
9. A.L. Ruoff, T.A. Grzybowski, in: S. Minomura (Ed.), Solid State Physics Under Pressure, Terra Scientific, Tokyo, 1985.

10. K.L. Heng, S.G. Chua, P. Wu, Chem. Mater. 12 (2000) 1648.
11. R. Khenata, M. Sahnoun, H. Baltache, M. Rerat, D. Rached, M. Driz, B. Bouhafs, Physica B 371 (2006)12.
12. A. Bouhemadou, R. Khenata, F. Zegrar, M. Sahnoun, H. Baltache, A.H. Reshak, Comput. Mater. Sci. 38 (2006) 263.
13. F. EI Haj Hassan, H. Akbarzadeh, Comput. Mater. Sci. 38 (2006) 362.
14. P. Bhardwaj, S. Singh, N.K. Gaur, Cent. Eur. J. Phys. 6 (2) (2008)223.
15. Y. Kaneko, T. Koda, J. Cryst. Growth 86 (1988) 72.
16. A. Pourghazi, M. Dadsetani, Physica B 370 (2005) 34.
17. M.P. Habas, R. Dovesi, A. Lichanot, J. Phys. Condens. Matter 10 (1998) 6897.
18. A.Pourghazi, M. Dadsetani, Physica B 370 (2005) 34.
19. S. Adachi, J. Appl. Phys. 61 (1987) 4869.

Ciation of this article