International Journal of Physical Research, 4 (2) (2016) 48-51

International Journal of Physical Research

Website: www.sciencepubco.com/index.php/IJPR
doi: 10.14419/ijpr.v4i2.6261
Research paper

Modified expression for calculating refractive index of A^NB^{8-N} type binary semiconductors

A. Latreche [1]*, S. Daoud [2]

[1] *Département des sciences de la matière, Université Mohamed Elbachir El Ibrahimi de Bordj Bou Arreridj, Bordj Bou Arreridj, 34000, Algeria*
[2] *Laboratoire Matériaux et Systèmes Electroniques (LMSE), Université Mohamed Elbachir El Ibrahimi de Bordj Bou Arreridj, Bordj Bou Arreridj, 34000, Algeria*
**Corresponding author E-mail: hlat26@yahoo.fr*

Abstract

In their recent work, Bahadur and Mishra proposed a new simple formula between the high-frequency refractive index and optical electronegativity difference, which has been established for large number of A^NB^{8-N} type binary semiconductors (groups: I-VII, II-VI, III-V and IV-VI.). In the present work, we have improved their expression by addition a correction term in their proposed formula. The minimum average percentage deviation in the present approach reveals that the modified Bahadur relation proves its identity and soundness compared to that of Bahadur's and others authors' relations.

Keywords: *Refractive Index; Electronegativity Difference; A^NB^{8-N} Type Binary Semiconductors.*

1. Introduction

Several models [1-10] based on quantum mechanics and oscillatory theory or upon experimental data have been elaborated with the fundamental aim of trying to relate the refractive index and the optical energy gap (E_g) of materials. Recently, some authors [11-14] have proposed models correlate the refractive index with the electronegativity difference which is a very useful parameter in understanding the nature of chemical bonding and predicting several important physical parameters.
In their work, Bahadur and Mishra [11] proposed an interesting simple formula between the high-frequency refractive index and electronegativity difference, which has been established for large number of A^NB^{8-N} type binary semiconductors (groups: I-VII, II-VI, III-V and IV-VI.). However, the authors, during the analysis of their work they did not distinguish between the two concepts of optical energy gap (E_g) and the Penn gap energy (E_p), which also called bonding-antibonding energy gap. In the present work, we propose a modified formula by respecting the correct notions of the optical energy gap and the Penn gap energy.

2. Theory and calculation

The correlation between energy gap (Eg) and optical electronegativity (ΔX^*) has been enlightened by Duffy [15, 16] in various binary systems and which reads as follows

$$E_g = 3.72\,(\Delta X^*) \tag{1}$$

In their works Singh et al. [7] correlated the refractive index n (electronic dielectric constant ε_∞) and Penn gap energy (E_p) as

$$n^2 = \varepsilon_\infty = 1 + bE_p^S \tag{2}$$

Where b and S are the ion characteristic constant and the family characteristic constant, respectively.
Bahadur and Mishra [11] thought that the definition of the E_p in-equation (2) and the definition of E_g in equation (1) are the same. First, they took the expression of E_g from the equation (1), then they substituted it into the equation (2), finally, they obtained a relation between the refractive index n and the optical electronegativity difference ΔX^*, their formula is given by the following expression [11]:

$$n = k\,(\Delta X^*)^\gamma \tag{3}$$

Where k and γ = -0.32 are constants.
It's important to note that, there is a difference between the energy gap (E_g) mentioned in the equation (1) and the Penn gap energy (E_p) mentioned in equation (2). The first one is named also the optical energy gap (E_g), and the second one is usually called the Penn gap (E_P) [8], [17], it called also the bonding-antibonding energy gap E_p (B-A).
The bonding-antibonding energy gap E_p ($_{A-B}$) is typically much larger than the optical energy gap E_g [18].
Gopal [17] has assumed a linear relation between the Penn gap, E_p, and the optical energy gap E_g as

$$E_p = E_g + K \tag{4}$$

Where K is a constant.
In order to conserve the originality of Bahadur's work [11] we follow exactly the same analysis that followed by Bahadur during the process of simplification.

From equations (1) and (4) the equation (2) can be rewritten

$$\left(\frac{n^2-1}{b}\right)^{1/S} = 3.72(\Delta X^*) + K \quad (5)$$

$\Delta X^* + C = \left(\frac{n^2-1}{c}\right)^{1/S}$, where c = b3.72^S and C=K/3.72 are constants.

$$\Delta X^* + C = c^{-1/S} n^{2/S}\left[1-\frac{1}{n^2}\right]^{1/S},$$
$$\Delta X^* + C = c^{-1/S} n^{2/S}\left[1-\frac{1}{Sn^2}+...\right], \quad (6)$$

Using binomial expansion up-to the second term since $1/n^2 << 1$.

$$\Delta X^* + C = c^{-1/S} n^{2/S} - \frac{1}{Sc^{1/S}} n^{-2\left(1-\frac{1}{S}\right)}, \quad (7)$$

$$\Delta X^* + C = l n^m + l' n^{m'}$$

Where $l = c^{-1/S}$, $l' = \frac{-1}{Sc^{1/S}}$ and $m = \frac{2}{S}$ $m' = -2\left(1-\frac{1}{S}\right)$.

Employing values of constants, the contribution due to second term, $l' n^{m'}$ is found negligible (The negligible term $l' n^{m'}$ can be added to the constant C, which is not negligible) and hence

$$\Delta X^* + C = l n^m$$

$$n = \frac{1}{l^{1/m}}\left(\Delta X^* + C\right)^{1/m} \quad (8)$$

$$n = k\,(\Delta X^* + C)^{\gamma} \quad (9)$$

Where the parameters k, C and γ are slightly, dependent on the nature group of material. The equation (9) is almost similar to that proposed by Salam [12].

$$n = F\,(\Delta X^* - D)^{-0.25} \quad (10)$$

Where F is dependent on the material group and D is unique numerical constant.

By optimizing known values of refractive index (n) and electronegativity difference (ΔX^*) data in regression software we have obtained the values of these constants for each group of material. The obtained values of k, C and γ are listed in Table 1.

Table 1: Numerical Values of the Constants K, C and γ for Different Material Groups.

	Group I-VII	Group II-VI	Group III-V	Group IV-VI
k	2.64	2.35	2.36	4.08
C	0.74	-0.04	-0.13	0.13
γ	- 0.48	-0.26	-0.22	-0.41

The present calculated and known values of refractive index have been presented in Table 2, and compared to the Bahadur's results [11]. As shown in Table 2, our proposed model gives better results than the Bahadur's results. The minimum average percentage deviation (3.17%) obtained in the present study, indicates the soundness of the present approach.

The calculated refractive index from equation (9) has been utilized to evaluate the electronic polarizability (α_e) by applying the Lorentz-Lorentz formula [19] as:

$$\alpha_e = \frac{n^2-1}{n^2+2}\frac{M}{d} 3.95x10^{-25} cm^3 \quad (11)$$

Where M and d are molecular weight and density of compounds, respectively. The present calculated and known values of electronic polarizability have been presented in Table 3 and compared to the Bahadur's results [11]. Our calculated values of electronic polarizability are in good agreement with the experimental values and the error calculations (5.19%) show a good precision than Bahadur's error calculations (5.38%).

Table 2: Refractive Index N of Different Material Groups. (The Known Values of n are taken from the Ref [11])

Comp-ounds	ΔX^* Ref [11]	Known Values Ref [11]	Bahadur Ref [11]	Present Work Eq.(07)
I-VII				
LiF	3	1.39	1.41	1.4
LiCl	2	1.66	1.6	1.63
LiBr	1.8	1.78	1.66	1.69
LiI	1.5	1.95	1.76	1.79
NaF	3.1	1.34	1.39	1.38
NaCl	2.1	1.54	1.58	1.6
NaBr	1.9	1.64	1.63	1.66
NaI	1.6	1.77	1.72	1.76
KF	3.2	1.36	1.38	1.37
KCl	2.2	1.49	1.55	1.57
KBr	2	1.56	1.6	1.63
KI	1.7	1.68	1.69	1.72
RbF	3.2	1.4	1.38	1.37
RbCl	2.2	1.49	1.55	1.57
RbBr	2	1.55	1.6	1.63
RbI	1.7	1.65	1.69	1.72
CsF	3.3	1.48	1.36	1.35
CsCl	2.3	1.61	1.53	1.55
CsBr	2.1	1.67	1.58	1.6
CsI	1.8	1.79	1.66	1.69
CuF	2.1	1.58	1.58	1.6
CuCl	1.1	1.93	1.94	1.97
CuBr	0.9	2.1	2.07	2.08
CuI	0.6	2.35	2.36	2.29
AgF	2	1.7	1.6	1.63
AgCl	1	2	2	2.02
AgBr	0.9	2.15	2.07	2.08
AgI	0.6	2.22	2.36	2.29
II-VI				
MgO	1.93	1.63	1.94	1.99
MgS	1.27	2.26	2.22	2.23
MgSe	1.2	2.43	2.26	2.26
MgTe	0.79	2.65	2.59	2.53
CaO	2.5	1.82	1.79	1.86
CaS	1.5	2.12	2.11	2.13
CaSe	1.4	2.26	2.16	2.17
SrO	2.5	1.8	1.79	1.86
SrS	1.5	2.1	2.11	2.13
SrSe	1.4	2.21	2.16	2.17
SrTe	1.1	2.41	2.33	2.31
BaO	2.55	1.98	1.78	1.85
BaS	1.6	2.15	2.06	2.09
BaSe	1.5	2.27	2.11	2.13
ZnO	1.9	2	1.95	2
ZnS	0.9	2.39	2.48	2.44
ZnSe	0.8	2.43	2.58	2.52
ZnTe	0.5	2.7	3	2.88
CdO	0.67	2.68	2.73	2.65
CdS	0.9	2.38	2.48	2.44
CdSe	0.86	2.44	2.52	2.47
CdTe	0.38	3.23	3.27	3.11
III-V				
AlN	1.43	2.2	2.12	2.23
AlP	0.6	2.75	2.8	2.79

AlAs	0.5	2.92	2.97	2.94
AlSb	0.4	3.19	3.19	3.15
GaN	1.4	2.24	2.14	2.24
GaP	0.5	2.9	2.97	2.94
GaAs	0.37	3.3	3.27	3.23
GaSb	0.24	3.75	3.76	3.84
InN	1.26	2.35	2.21	2.3
InP	0.41	3.1	3.17	3.12
InAs	0.3	3.51	3.5	3.49
InSb	0.23	3.96	3.81	3.92
IV-VI				
SnS	0.7	4.42	4.48	4.4
SnSe	0.6	4.79	4.71	4.64
PbS	0.7	4.15	4.48	4.4
PbSe	0.6	4.78	4.71	4.64
PbTe	0.3	5.73	5.88	5.77
Average percentage deviation			3.53 %	3.17%

Table 3: Electronic Polarizability α_e of Different Material Groups. (The Known Values of α_e are Taken from the Ref [11])

Comp-ounds	Mol. Weight [11]	Density [g/cm3] [11]	Electronic polarizability [10^{-24} cm^3] Known values [11]	Bahad [11]	Present work
LiF	25.937	2.64	0.89	0.96	0.94
LiCl	42.392	2.07	2.98	2.78	2.87
LiBr	86.843	3.46	4.12	3.65	3.78
LiI	133.843	3.49	6.15	6.21	6.43
NaF	41.988	2.56	1.15	1.54	1.51
NaCl	58.443	2.17	3.24	3.53	3.64
NaBr	102.894	3.2	4.38	4.51	4.67
NaI	149.894	3.67	6.41	6.38	6.61
KF	58.1	2.48	1.99	2.14	2.08
KCl	74.555	1.98	4.08	4.77	4.90
KBr	119.006	2.75	5.22	5.86	6.06
KI	166.006	3.13	7.25	7.99	8.28
RbF	104.468	3.56	2.54	2.67	2.60
RbCl	120.923	2.8	4.63	5.47	5.62
RbBr	165.374	3.35	5.77	6.69	6.91
RbI	212.374	3.55	7.8	9.01	9.34
CsF	151.903	4.12	3.6	3.25	3.14
CsCl	168.358	3.99	5.69	5.17	5.30
CsBr	212.809	4.44	6.83	6.28	6.47
CsI	259.809	4.51	8.86	8.37	8.67
CuF	82.54	4.23	2.57	2.56	2.64
CuCl	98.99	4.14	4.5	4.53	4.63
CuBr	143.45	4.98	6.05	5.94	5.99
CuI	190.44	5.62	8.05	8.06	7.86
AgF	126.87	5.85	3.31	2.94	3.04
AgCl	143.32	5.56	5.09	5.09	5.17
AgBr	187.78	6.47	6.27	5.99	6.03
AgI	234.77	6	8.76	9.31	9.07
MgS	56.38	2.84	4.53	4.45	4.46
MgSe	103.27	4.21	6	5.61	5.60
MgTe	151.91	4.54	8.82	8.66	8.50
CaO	56.08	3.32	2.9	2.83	3.00
CaS	72.14	2.5	6.13	6.09	6.17
CaSe	119.04	3.57	7.62	7.22	7.28
SrO	103.62	4.7	3.72	3.69	3.92
SrS	119.68	3.7	6.8	6.83	6.91
SrSe	166.58	4.38	8.47	8.24	8.30
SrTe	215.22	4.83	10.84	10.48	10.42
BaO	153.34	5.72	5.22	4.44	4.73
BaS	169.4	4.25	8.61	8.20	8.34
BaSe	216.3	5.02	9.88	9.10	9.21
ZnO	81.37	5.61	2.86	2.78	2.86
ZnS	97.43	3.98	5.91	6.12	6.03
ZnSe	144.33	5.42	6.53	6.87	6.75
ZnTe	192.97	6.34	8.14	8.74	8.51
CdS	144.46	4.82	7.2	7.49	7.38
CdSe	191.36	5.51	8.1	8.79	8.65
AlN	40.99	3.26	2.79	2.68	2.83
AlP	57.96	2.85	5.51	5.59	5.56
AlAs	101.9	3.81	7.55	7.64	7.58
AlSb	148.73	4.22	10.49	10.49	10.41
GaN	83.73	6.1	3.1	2.95	3.10
GaP	100.69	4.13	6.85	6.96	6.91
GaAs	144.64	5.32	8.24	8.20	8.15
GaSb	191.47	5.62	10.94	10.95	11.04
InN	128.83	6.88	4.45	4.17	4.35
InP	145.79	4.79	8.92	9.02	8.95
InAs	189.74	5.66	10.47	10.45	10.43
InSb	236.57	5.78	13.42	13.23	13.37
SnS	150.75	5.22	9.82	9.86	9.81
SnSe	197.65	6.18	11.11	11.07	11.02
PbS	239.26	7.61	10.48	10.73	10.68
PbSe	286.15	8.15	12.19	12.15	12.10
PbTe	334.79	8.16	14.81	14.88	14.83
Average percentage deviation				5.38%	5.19%

3. Conclusion

In this short paper, we have improved the Bahadur and Mishra approach by adding a correction term to their formula. This novel correlation between optical refractive index and electronegativity difference gives better agreement with the experimental values than the models proposed by earlier workers, which in turn demonstrate the soundness of the present model.

References

[1] T.S. Moss, A Relationship between the Refractive Index and the Infra-Red Threshold of Sensitivity for Photoconductors, Proceedings of the Physical Society. Section B, Vol.63, No.3, (1950) pp. 167-176. http://dx.doi.org/10.1088/0370-1301/63/3/302

[2] T.S. Moss, Relations between the Refractive Index and Energy Gap of Semiconductors, Physical Status Solidi B, Vol.131, No.2, (1985) pp.415-427. http://onlinelibrary.wiley.com/doi/10.1002/pssb.2221310202/abstract. http://dx.doi.org/10.1002/pssb.2221310202.

[3] N.M. Ravindra & V.K. Srivastava, Variation of refractive index with energy gap in semiconductors, Infrared Physics. Vol.19, No.5, (1979) pp.603-604. http://dx.doi.org/10.1016/0020-0891(79)90081-2.

[4] V.P. Gupta & N.M. Ravindra, Comments on the Moss Formula, Physical Status Solidi B, Vol.100, No.2, (1980) pp. 715-719. http://dx.doi.org/10.1002/pssb.2221000240.

[5] P. Herve & L.K.J. Vandamme, General relation between refractive index and energy gap in semiconductors, Infrared Physics & Technology. Vol.35, No.4, (1994) pp. 609-615. http://dx.doi.org/10.1016/1350-4495(94)90026-4.

[6] R. R. Reddy &Y. Nazeer Ahammed, A study on the Moss relation, Infrared Physics & Technology. Vol.36, No.5, (1995) pp. 825-830. http://dx.doi.org/10.1016/1350-4495(95)00008-M.

[7] R.P. Singh, P. Singh & K.K. Sarkar, Correlation between the refractive index and the energy gap of simple and complex binary compounds-II, Infrared Physics. Vol.26, No.3, (1986) pp. 167 169-. http://dx.doi.org/10.1016/0020-0891(86)90019-9.

[8] R.P. Singh, P.P. Singh & K.K. Sarkar, "Correlation between the refractive index and the energy gap of simple and complex binary compounds", Infrared Physics. 26, No.1, (1986) pp. 1-3. http://dx.doi.org/10.1016/0020-0891(86)90039-4.

[9] M. Anani, C. Mathieu, S. Lebid, Y. Amar, Z. Chama & H. Abid, Model for calculating the refractive index of a III-V semiconductor, Computational Materials Science, Vol.41, No.4, (2008), pp. 570-575. http://dx.doi.org/10.1016/j.commatsci.2007.05.023.

[10] V. Kumar & J. K. Singh, Model for calculating the refractive index of different materials, Indian Journal of Pure and Applied Physics, Vol.48, (2010), pp. 571-574. http://www.nusod.org/piprek/guden96msmse.pdf.

[11] A. Bahadur & M. Mishra, " Correlation Between Refractive Index and Electronegativity Difference for A^NB^{8-N} Type Binary Semiconductors", Acta Physica Polonica A, Vol.123, No.4, (2013) pp. 737-740. http://dx.doi.org/10.12693/APhysPolA.123.737.

[12] M. A. Salem, The dependence of the high frequency refractive index on the electronegativities in compound semiconductors, Chinese Journal of Physics. Vol.41, No.3, (2003) pp. 288-295.

[13] B. P. Singh, S. Tripti & V. Singh, "Analysis of optoelectronic properties of A^NB^{8-N} type binary solids", Indian Journal of Pure and Applied Physics, Vol.46, No.7, (2008) pp. 502-506.

[14] R.R. Reddy, K. Rama Gopal, K. Narasimhulu, L. Siva Sankara Reddy, K. Raghavedra Kumar, C.V. Krishna Reddy, S.N. Ahmed, Correlation between optical electronegativity and refractive index of ternary chalcopyrites, semiconductors, insulators, oxides and alkali halides, Optical Materials. Vol.31, No.2, (2008) pp. 209-212. http://dx.doi.org/10.1016/j.optmat.2008.03.010.

[15] J. A. Duffy, Trends in energy gaps of binary compounds: an approach based upon electron transfer parameters from optical spectroscopy, Journal of Physics C: Solid State Physics, Vol.13, No.16, (1980) pp. 2979-2989. http://dx.doi.org/10.1088/0022-3719/13/16/008.

[16] J.A. Duffy, *Bonding Energy Levels and Bonds in Inorganic Solids*, Longman Scientific & Technical, England (1990). ISBN 0470215674, 9780470215678.

[17] V. Gopal, Energy gap-refractive index interrelation, Infrared Physics. Vol.22, No.5, (1982) pp. 255-257. http://dx.doi.org/10.1016/0020-0891(82)90052-5.

[18] J. I. Gersten and F. W. Smith, *The physics and chemistry of materials*, New York, John Wiley & Sons, INC, (2001). ISBN 10: 0471057940, ISBN 13: 9780471057949

[19] A.K. Jonscher, *Dielectric Relaxation in Solids*, Chelsea Dielectric Press, London (1983). ISBN 0095087109, 9780095087100