

Model for calculating refractive index from energy gap for binary and ternary chalcopyrite semiconductors

Umar Farooque^{1,*}, Tarique Rashid², Ajay Kumar¹, Shadab Rabbani¹, Faiz Ahmad³

¹Department of Electronics and Communication Engineering, Muzaffarpur Institute of Technology, Muzaffarpur, Bihar, 842003, India

²Department of Electrical and Electronics Engineering, Darbhanga College of Engineering Darbhanga, Bihar, 846005, India

³Department of Electrical Engineering, Muzaffarpur Institute of Technology, Muzaffarpur, Bihar, 842003, India

*Email: ufarooque@mitmuzaffarpur.org

Received: 10 March 2023; Accepted for publication: 8 July 2023

Abstract. Based on the energy gap (E_g) data, a simple model has been proposed for the calculation of refractive index (n) of the binary semiconductors, oxides, halides, insulators, and ternary chalcopyrite semiconductors of $A^I B^{III} C_2^{VI}$, and $A^{II} B^{IV} C_2^V$ families. The refractive index values of the above-mentioned semiconductor materials have been calculated by utilizing the proposed model. Further, the reported values of the refractive index by different models in the literature for the considered semiconductor materials have also been mentioned for the comparison purpose. Moreover, the values of the average percentage deviations have been calculated for all models. The obtained values of the average percentage deviation for the proposed model is almost lowest compared to that of the reported models. Additionally, most of the reported models have not mentioned the values of refractive index for different semiconductor materials, while the proposed model has been utilized to calculate the values of refractive index for a wide range of semiconductor materials. Thus, it validates the suitability of our proposed model in the estimation of refractive index values of different technologically important materials.

Keywords: Binary, ternary chalcopyrite, semiconductors, refractive index, energy gap.

Classification numbers: 2.1.1, 2.1.3, 2.2.2

1. INTRODUCTION

The refractive index (n) and the energy gap (E_g) are the two important parameters that are used to describe the electronic and optical properties of the binary semiconductors, oxides,

halides, insulators, and ternary chalcopyrite semiconductors. The chalcopyrite semiconductor structures having body-centered tetragonal unit cells result from their respective binary components in the cubic zinc-blende structures, by doubling the unit cell along c [1]. They are classified into two families, namely, $I - III - VI_2$ compounds

$$(I = Cu, Ag; III = B, Al, Ga, In; VI = S, Se, Te)$$

and $II - IV - V_2$ compounds

$$(II = Zn, Cd; IV = Si, Ge, Sn; V = N, P, As, Sb) [2].$$

These chalcopyrite semiconductor materials are promising materials for the spintronics application due to their ability to host ferromagnetism at room temperature [1]. Further, due to the large non-linear coefficient, large area growth availability, and birefringence property of zinc-based chalcopyrites $ZnXPn_2$ ($X = Si, Ge, Sn$; $P_n = P, As, Sb$), these chalcopyrite semiconductor materials are suitable for nonlinear optical device applications [3]. Moreover, apart from these, the chalcopyrite semiconductors have potential applications in optical sources and detectors, integrated optoelectronic devices, and other linear and nonlinear optical devices [4 - 10].

The energy gap is related to the photon absorption threshold of the material, while the refractive index is a measure of the incident spectral radiation. The choice of the material for a specific device design depends critically upon the nature and values of the energy gap and refractive index. Therefore, precise calculation of the refractive index of different materials has been a topic of interest among researchers across the globe. Generally, an increase in energy gap results in a decrease in the refractive index value of a material, so there should be a correlation between these two quantities. Several efforts have been made to correlate refractive index and energy gap [8, 11 - 22], and optical electronegativity and refractive index [6, 23-25].

An analytical model is greatly desired to evaluate the refractive index of the new materials in the characterization of the device design whose experimental data are not known. Moreover, the analytical model is also required for the calculation of refractive index (n) value of a material from its energy gap (E_g) value. However, the analytical model should be such that the calculated value is close to the experimentally obtained value, at the same time the number of coefficients involved in the analytical model should be less to minimize the computational complexity.

Therefore, several attempts have been made to obtain an analytical model for the calculation of refractive index values from the energy gap values. Based on the scaling of energy levels by a factor of $\frac{1}{\epsilon_{opt}^2}$, where $\epsilon_{opt}(= n^2)$, represents the optical dielectric constant of materials,

Moss [11 - 13] proposed a relationship between refractive index and energy gap. A linear relationship between the refractive index and the energy gap has been proposed by other researchers [15 - 16]. Ravindra *et al.* [17] have modified the Moss formula and presented the relationship between refractive index and energy gap in the exponential form. Herve-Vandamme *et al.* [18] correlated the refractive index and energy gap. An empirical model has been developed by Anani *et al.* [19] for the estimation of refractive index from the energy gap. Kumar *et al.* [20] have reported a simple model for calculating the refractive index. Tripathi [21] and Kumar *et al.* [22] introduced exponential dependence of refractive index on the energy gap for different materials including ternary chalcopyrite semiconductors. Recently, in order to achieve high accuracy of the calculated values of refractive index, H. M. Gomaa *et al.* [8] have proposed a model for the calculation of refractive index using the experimental values of energy gap. Further, various models reported in the literature for the estimation of refractive index have been discussed in detail in [8, 21].

In this work, we propose a simple model for the calculation of refractive index from energy gap. The proposed model is simple in nature, because it requires only the values of the

two parameters, namely A and B , and it may be accessible to calculate the values of the refractive index for a wide range of binary semiconductors, oxides, halides, insulators, and ternary chalcopyrite semiconductor materials. Further, the average percentage deviation of the proposed model has been calculated and compared with that of the other models. Except Kumar *et al.* [22], none of the other reported works have considered all the materials mentioned in Table 1 and Table 2 in their investigations. Further, the value of the average percentage deviation for the binary semiconductors, oxides, halides, and insulators in Table 1 is significantly large for the Kumar *et al.* [22] model compared to the value obtained in the proposed model. Meanwhile, for the ternary chalcopyrite semiconductors, the value of the average percentage deviation is slightly higher in the case of the proposed model compared to Kumar *et al.* [22] model. The calculated values by utilizing the proposed model are in fairly good agreement with the experimental and the reported values in the literature, which validates the suitability of our proposed model in the estimation of refractive index values of different technologically important materials.

2. MATERIALS AND METHODS

2.1. Calculation of refractive index of binary semiconductors

In this section, we have presented a brief description of the various models proposed by earlier workers starting from Moss [11] for the estimation of refractive index (n) of different material groups.

Moss [11] relation

$$n^4 = \frac{95}{E_g}, \quad (1)$$

Ravindra *et al.* [15] relation

$$n = 4.084 - 0.62E_g, \quad (2)$$

Ravindra *et al.* [17] relation

$$n^4 = \frac{108}{E_g}, \quad (3)$$

Herve-Vandamme *et al.* [18] relation

$$n^2 = 1 + \left(\frac{13.6}{E_g + 3.4}\right)^2, \quad (4)$$

Kumar *et al.* [20] relation

$$n = 3.3668E_g^{(-0.32234)}, \quad (5)$$

Tripathi [21] relation

$$n = 1.73(1 + 1.9017\exp[-0.539E_g]), \quad (6)$$

Kumar *et al.* [22] relation

$$n = 3.892\exp[-0.16E_g], \text{ and} \quad (7)$$

H. M. Gomaa *et al.* [8] relation

$$n = \left(\frac{A}{E_g^{0.5}} - B\right)^{\frac{1}{2}}, \quad (8)$$

where, $A = 3.44^2$ and $B = 3.44^{\frac{1}{2}}$

Based on the above, we propose the following relation for ' n '

$$n = \left(1 + \frac{A}{E_g + B}\right), \quad (9)$$

where, A and B are the constants and their simulated values are 5.234 and 0.9468, for the binary semiconductors, respectively. The values of constants A and B have been obtained by utilizing

the experimental values of the energy gap and refractive index in the proposed model and by optimization using the regression platform.

2.2. Calculation of refractive index of ternary chalcopyrite semiconductors

Ternary chalcopyrite semiconductors are materials of technological interest due to their potential applications in optoelectronic, photovoltaic, and optical devices. Recently, several attempts have been made to study the various properties of these semiconductors [3, 21-22, 27]. Tripathi [21] and Kumar *et al.* [22] have calculated the refractive index of these materials using Equations 6 and 7, respectively. Meanwhile, recently in [27], the electronic, optical, and structural properties of AgTiX_2 ($\text{X} = \text{S, Se, Te}$) chalcopyrite semiconductors have been studied. In this section, the work has been extended to calculate the values of refractive index of the ternary chalcopyrite semiconductors of $A^I B^{III} C_2^{VI}$, and $A^{II} B^{IV} C_2^V$ families. The simulated values of constants A and B have been obtained as 9.420 and 3.229, for the ternary chalcopyrite semiconductors, respectively.

3. RESULTS AND DISCUSSION

Using the proposed model, i.e., Eq. 9, and the experimental values of the energy gap [26], we have calculated the values of the refractive indices and presented them in Table 1, along with the values reported from other models for binary semiconductors, oxides, halides, and insulators. In order to obtain the fitness of the proposed model, the values of average percentage deviation have been calculated for all the models and given in the bottom row of Table 1. From Table 1, it has been observed that there is a significant reduction in the value of average percentage deviation utilizing the proposed model compared to the earlier reported models. The obtained value of the average percentage deviation by the proposed model is 7.7992, which is the lowest compared to those obtained by the other reported models. Further, different models have been analyzed, showing that as the value of energy gap approaches ‘infinity’ theoretically, the respective value of refractive index approaches ‘zero’ in the models reported by different workers [11 - 13, 20, 22], ‘negative value’ in Ravindra *et al.* [15] model, ‘1.73’ in Tripathi [21] model, and ‘imaginary value’ in H. M. Gomaa *et al.* [8] model compared to the value ‘1’ in the proposed model and the model reported by Herve-Vandamme *et al.* [18]. Moreover, as compared to the proposed model, the Herve-Vandamme *et al.* [18] model underestimates the value of refractive index for lower values of energy gap and the average percentage deviation is also high. On the other hand, the ‘negative value’ in the Ravindra *et al.* [15] model and ‘imaginary value’ in [8] show that these equations require correction. Therefore, it is concluded that the value of the refractive index calculated utilizing the proposed model is close to the experimental value and hence, the proposed model is a suitable choice for the calculation of refractive index values from the energy gap data compared to the other reported models.

To gain a better insight into the fitness of the different models, plots between the calculated/reported refractive index values as a function of energy gap for the considered semiconductor materials mentioned in Table 1 are shown in Figure 1. The success and limitations of the previously reported models have been discussed in detail by Tripathi [21]. Further, it has been claimed that the values of refractive index calculated utilizing the empirical exponential relation reported in [21] are in good agreement with the known values over a broad range of energy gap values. However, it can be observed from Table 1 that the value of average percentage deviation of the model reported by Tripathi [21] is 9.3021, while for the proposed model it is 7.992. On the other hand, the number of parameters involved in the model reported

by Tripathi [21] is three, while in the proposed model only two parameters are required, which minimizes the computational complexity.

Table 1. Refractive index of binary semiconductors, oxides, halides, and insulators.

Material	Eg (eV) Expt. [26]	Refractive Index (n)								
		Expt. [26]	This work Eq. (9)	Tripathi [21]	Kumar <i>et al.</i> [20]	Kumar <i>et al.</i> [22]	Moss [11]	Ravindra <i>et al.</i> [15-16]	Herve-Vandamme <i>et al.</i> [18]	H. M. Gomaa <i>et al.</i> [8]
GeTe	0.1	6	6	4.8473	7.0722	5.6257	5.5518	4.0220	3.9386	5.9640
InSb	0.235, 0.17#	5.13	5.4288	4.6285	5.3697	4.9068	4.4840	3.9383	3.8045	5.1810
PbSe	0.278, 0.28#	4.59	5.2734	4.5621	5.0866	4.7767	4.2995	3.9116	3.7639	4.5290
PbTe	0.311	5.35	5.1612	4.5122	4.9059	4.6917	4.1806	3.8912	3.7334	4.4040
InAs	0.417, 0.35#	4.1	4.8378	4.3577	4.4634	4.4766	3.8851	3.8255	3.6389	4.2600
Ge	0.664	4.052	4.2493	4.0301	3.8418	4.1555	3.4585	3.6723	3.4384	3.5650
GaSb	0.812, 0.73#	3.82	3.9759	3.8538	3.6006	4.0239	3.2888	3.5806	3.3298	3.4630
Si	1.124	3.4777	3.5275	3.5251	3.2423	3.8199	3.0321	3.3871	3.1247	3.0540
GaAs	1.42, 1.43#	3.3	3.2114	3.2603	3.0070	3.6797	2.8600	3.2036	2.9555	2.8360
CdTe	1.56	2.817	3.0879	3.1491	2.9172	3.6247	2.7935	3.1168	2.8828	2.7600
AlSb	2.22	3.19	2.6528	2.7243	2.6036	3.4258	2.5577	2.7076	2.5909	2.4670
AlAs	2.153	2.87	2.6885	2.7609	2.6294	3.4426	2.5773	2.7491	2.6172	2.4930
GaP	2.26, 2.78#	3.2, 3.35#	2.6322	2.7031	2.5887	3.4160	2.5463	2.6828	2.5755	2.2900
ScN	2.26	2.61	2.6322	2.7031	2.5887	3.4160	2.5463	2.6828	2.5755	NA
ZnTe	2.3, 2.26#	2.962, 2.7#	2.6120	2.6823	2.5741	3.4064	2.5351	2.6580	2.5604	2.4530
CdS	2.5, 2.4#	2.38	2.5185	2.5850	2.5058	3.3613	2.4828	2.5340	2.4879	2.4050
CuBr	3	2.117	2.3261	2.3830	2.3628	3.2646	2.3722	2.2240	2.3278	2.2310
CuI	3.1	2.346	2.2934	2.3488	2.3379	3.2475	2.3528	2.1620	2.2989	NA
AlP	3.63, 2.45#	2.75	2.1436	2.1950	2.2220	3.1666	2.2618	1.8334	2.1608	2.3890
SiC	2.6	2.6	2.4757	2.5402	2.4743	3.3402	2.4586	2.4720	2.4536	2.3420
CuCl	3.3	1.97	2.2325	2.2855	2.2913	3.2152	2.3163	2.0380	2.2440	2.1520
GaN	3.299, 3.25#	2.4	2.2327	2.2858	2.2915	3.2154	2.3165	2.0386	2.2443	2.1700
ZnS	3.68	2.3505	2.1312	2.1826	2.2122	3.1596	2.2541	1.8024	2.1489	2.0770
BN	7.5, 4.6#	2.117	1.6196	1.7878	1.7585	2.8194	1.8865	N.A	1.5928	1.9140
ZnO	3.35	2.015	2.2181	2.2708	2.2802	3.2075	2.3076	2.0070	2.2308	2.1470
GeO ₂	5.6	1.6045	1.7995	1.8908	1.9322	2.9544	2.0295	0.6120	1.8023	1.7740
AlN	4.9, 3.8#	2.16	1.8952	1.9645	2.0172	3.0182	2.0984	1.0460	1.9079	2.0530
CsI	6.2	1.7806	1.7324	1.8464	1.8698	2.9066	1.9785	0.2400	1.7257	1.7020
CsBr	6.9	1.6929	1.6670	1.8098	1.8064	2.8573	1.9263	N.A	1.6492	1.6280
NaBr	7.5	1.64	1.6196	1.7878	1.7585	2.8194	1.8865	N.A	1.5928	1.5700
CsCl	7.4	1.64	1.6271	1.7909	1.7662	2.8255	1.8929	N.A	1.6017	1.5800
KBr	7.6	1.5566	1.6124	1.7847	1.7510	2.8135	1.8803	N.A	1.5841	1.5610
KCl	8.5	1.4879	1.5541	1.7637	1.6890	2.7635	1.8284	N.A	1.5136	1.4850
SiO ₂	8.4	1.56	1.5600	1.7656	1.6955	2.7688	1.8338	N.A	1.5208	1.4930
Avg. % Deviation			7.7992	9.3021	9.6144	35.8686	12.1378	43.5482	11.21	8.2262
N.A – Not Applicable, # Ref [8]										

In order to check the suitability of the proposed model, the refractive index values of the ternary chalcopyrite semiconductor materials have been estimated using the proposed model, i.e., Eq. 9, and the calculated values are listed in Table 2, along with the values reported by different models. Further, the average percentage deviations of the proposed model and reported models have been calculated and are mentioned in the bottom row of Table 2.

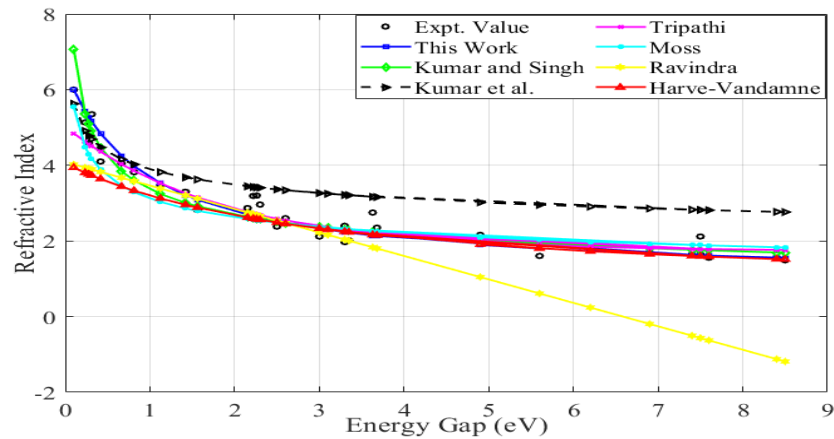


Figure 1. Energy gap dependent variation in refractive index values of semiconductors, oxides, halides, and insulators.

Table 2. Refractive index of ternary chalcopyrite semiconductors.

Ternary Chalcopyrite Semiconductor	Eg Expt. [22]	Refractive Index (n)								
		Expt. [22]	This work Eq. (9)	Kumar <i>et al.</i> [20]	Kumar <i>et al.</i> [22]	Tripathi [21]	Moss [11, 13]	Ravindra <i>et al.</i> [15]	Herve-Vandamme <i>et al.</i> [18]	H. M. Gomaa <i>et al.</i> [8]
CdSnAs ₂	0.26	3.7	3.6999	5.1975	3.7334	4.5897	4.3721	3.9228	3.7808	4.621
CdGeAs ₂	0.61	3.4	3.4796	4.0356	3.5528	4.1497	3.5930	3.7306	3.5117	3.646
CuInTe ₂	0.95	3.4	3.3794	3.7263	3.4630	3.9498	3.3775	3.6314	3.3890	3.207
AgInTe ₂	0.99	3.4	3.2925	3.5084	3.3808	3.7774	3.2234	3.5384	3.2825	NA
CuGaTe ₂	0.997, 1#	3.3	3.2487	3.4114	3.3378	3.6910	3.1540	3.4888	3.2287	3.159
ZnSnAs ₂	1, 0.65#	3.6	3.2487	3.4114	3.3378	3.6910	3.1540	3.4888	3.2287	3.581
CuInSe ₂	1.038, 0.96#	2.9	3.2275	3.3668	3.3165	3.6491	3.1220	3.4640	3.2026	3.197
AgGaTe ₂	1.09	3.3, 3.46#	3.2275	3.3668	3.3165	3.6491	3.1220	3.4640	3.2026	3.070
ZnGeAs ₂	1.15, 0.85#	3.5	3.2066	3.3245	3.2954	3.6082	3.0915	3.4392	3.1770	3.314
CdSnP ₂	1.16, 1.17#	3.1	3.1512	3.2185	3.2379	3.5001	3.0148	3.3710	3.1089	3.014
AgInSe ₂	1.23	3.32	3.1414	3.2007	3.2275	3.4811	3.0018	3.3586	3.0969	NA
CuInS ₂	1.499	2.6	3.1221	3.1662	3.2070	3.4437	2.9767	3.3338	3.0732	2.794
CdSiAs ₂	1.54, 1.55#	3.5	2.9711	2.9232	3.0372	3.1568	2.7980	3.1230	2.8878	2.766
ZnSnP ₂	1.65, 1.62#	2.9	2.9711	2.9232	3.0372	3.1568	2.7980	3.1230	2.8878	2.728
ZnSiAs ₂	1.69, 1.7#	3.1, 2.8#	2.9268	2.8594	2.9842	3.0746	2.7505	3.0548	2.8334	2.687
CuGaSe ₂	1.69, 1.7#	2.8	2.9111	2.8375	2.9651	3.0460	2.7341	3.0300	2.8142	2.687
CdGeP ₂	1.71, 1.72#	3.3	2.9034	2.8268	2.9557	3.0319	2.7261	3.0176	2.8047	2.677
AgGaSe ₂	1.79, 1.8#	2.8	2.8620	2.7709	2.9041	2.9569	2.6842	2.9494	2.7540	2.639
ZnGeP ₂	1.98, 1.99#	3.1	2.8474	2.7516	2.8856	2.9307	2.6697	2.9246	2.7361	2.556
AgInS ₂	1.99, 1.86#	2.5	2.8049	2.6970	2.8307	2.8555	2.6286	2.8502	2.6841	2.612
CuAlTe ₂	2.05, 0.9#	3.3	2.7677	2.6507	2.7813	2.7907	2.5934	2.7820	2.6385	3.259
ZnSiP ₂	2.09	3.1	2.7644	2.6466	2.7769	2.7850	2.5904	2.7758	2.6344	2.512
AgAlTe ₂	2.26	2.54	2.7130	2.5850	2.7067	2.6979	2.5435	2.6766	2.5717	NA
CuGaS ₂	2.39, 2.4#	2.67, 2.38#	2.6646	2.5288	2.6383	2.6179	2.5005	2.5774	2.5127	2.405

CdSiP2	2.44, 2.2#	3.1	2.6587	2.5222	2.6298	2.6084	2.4954	2.5650	2.5055	2.475
AgAlSe2	2.54	2.47	2.6300	2.4898	2.5881	2.5623	2.4706	2.5030	2.4706	NA
CuAlSe2	2.69	2.6	2.5888	2.4444	2.5267	2.4976	2.4355	2.4100	2.4204	2.312
AgGaS2	2.69	2.4, 2.6#	2.5835	2.4386	2.5187	2.4894	2.4310	2.3976	2.4140	2.312
CuAlS2	3.49	2.4	2.4814	2.3307	2.3587	2.3388	2.3472	2.1434	2.2904	2.114
MgGeP2	0.24	-	3.7155	N.A	3.74	N.A	N.A	N.A	N.A	N.A
BeGeP2	0.9	-	3.2814	N.A	3.37	N.A	N.A	N.A	N.A	N.A
MgSnAs2	0.93	-	3.2650	N.A	3.35	N.A	N.A	N.A	N.A	N.A
BeSiAs2	1.1	-	3.1760	N.A	3.26	N.A	N.A	N.A	N.A	N.A
BeSnAs2	1.15	-	3.1512	N.A	3.23	N.A	N.A	N.A	N.A	N.A
MgSnP2	1.56	-	2.9670	N.A	3.03	N.A	N.A	N.A	N.A	N.A
MgGeAs2	1.6	-	2.9507	N.A	3.01	N.A	N.A	N.A	N.A	N.A
BeGeAs2	1.68	-	2.9189	N.A	2.97	N.A	N.A	N.A	N.A	N.A
MgSiAs2	2	-	2.8015	N.A	2.82	N.A	N.A	N.A	N.A	N.A
MgSiP2	2		2.8015	N.A	2.82	N.A	N.A	N.A	N.A	N.A
MgGeP2	2.1	-	2.7677	N.A	2.78	N.A	N.A	N.A	N.A	N.A
BeSnP2	1.98	-	2.8084	N.A	2.83	N.A	N.A	N.A	N.A	N.A
Avg. % Deviation			5.9854	8.1338	5.9024	9.3859	8.1379	7.3494	6.6458	9.8430
N.A – Not Applicable, # Ref [8]										

From Table 2, it can be observed that except Kumar *et al.* [22], none of the other reported works have considered all the materials in their investigations. Further, the value of the average percentage deviation of the proposed model is 5.9854, which is slightly greater than that of the Kumar *et al.* [22] model. Meanwhile, for the semiconductor materials mentioned in Table 1, the average percentage deviation value for the Kumar *et al.* [22] model is 35.8686, which is significantly larger than the value of 7.7992 obtained in the proposed model. This validates the suitability of the proposed model for a wide range of semiconductor materials compared to the other reported models.

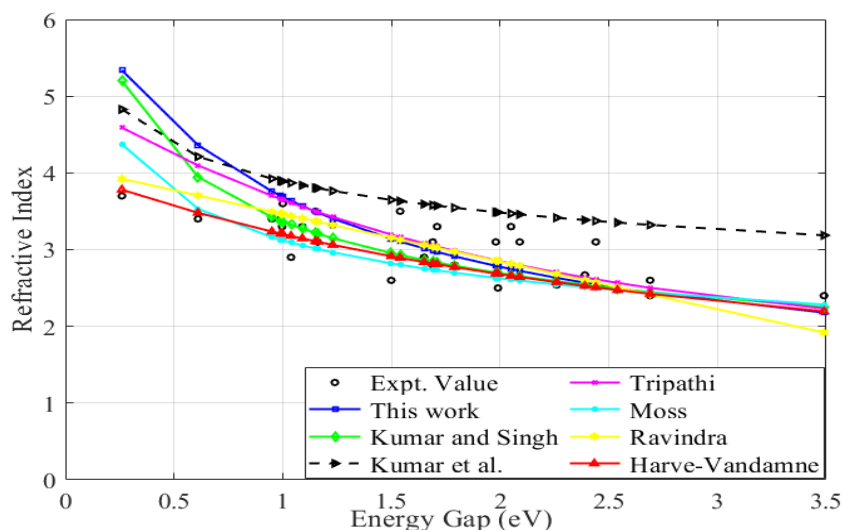


Figure 2. Energy gap dependent variation in refractive index values of ternary chalcopyrite semiconductors.

For the better understanding of the fitness of different models, plots between the calculated/reported values of the refractive index as a function of energy gap for the ternary chalcopyrite semiconductor materials are shown in Fig. 2. From Fig. 2, it can be observed that the results obtained using the proposed model follow the trend of variation in experimental values of refractive index and also are in reasonable agreement with the experimental values.

4. CONCLUSIONS

A simple model has been proposed for the estimation of refractive index as a function of energy gap of various materials, such as, binary semiconductors, oxides, halides, insulators, and ternary chalcopyrite semiconductors. The calculated refractive index values of 34 materials are shown in Table 1 and the curve between energy gap and refractive index plotted is shown in Figure 1. The average percentage deviations of the proposed model and earlier models have been

calculated using the relation $Avg. \% Dev. = \left[\frac{|(n_{expt.} - n_{cal.})|}{(n_{expt.})} \right] \times 100$. The estimated

values of the average percentage deviation of the proposed model is 7.7992, compared to the values of 8.2262 [8], 9.3021 [21], 9.6144 [20], and 35.868 [22] from the earlier models, which shows that our calculated values are closer to the experimental values. Further, the proposed relation of refractive index has been modified to fit the experimental values of the refractive index for ternary chalcopyrite semiconductors. The calculated values are listed in Table 2 and plotted in Figure 2. The results obtained using the proposed model follow the variation trend of the experimental values of the refractive index and are also in reasonable agreement with the experimental values. In almost all reported models, for high values of the energy gap, the values of the refractive index are overestimated compared to the values obtained from the proposed model. The lower value of the average percentage deviation of the proposed model compared to the other models indicates that the values calculated from the proposed model are closer and best fit the experimental values, which establishes the effectiveness of the proposed model.

Acknowledgements. The authors are thankful to Professor V. Kumar, Indian Institute of Technology (Indian School of Mines), Dhanbad, for his immense support and encouragement to carry out this work.

CRedit authorship contribution statement. Umar Farooque, Tarique Rashid: carried out literature survey, and identified research problem, and based on that proposed a model, collected data from the literature and obtained data from the proposed model for Table 1 and 2, Shadab Rabbani and Faiz Ahmad: done Matlab simulation to plot Figures 1 and 2. Ajay Kumar: wrote the manuscript.

Declaration of competing interest. The authors declare that there are no competing financial and/or non-financial interests related to the submitted work.

REFERENCES

1. B. Sadhukhan, Y. Zhang, R. Ray, J. van den Brink, First-principles calculation of shift current in chalcopyrite semiconductor ZnSnP_2 , *Physical Review Materials* **4** (1-8) (2020) 064602.
2. S. Das, P. Ranjan, K. Gaurav, P. K. Surolia, T. Chakraborty, Structure, electronic and optical properties of chalcopyrite-type semiconducting materials XGaY_2 ($\text{X} = \text{Cu, Ag, Au}$; $\text{Y} = \text{S, Se, Te}$) for solar cell applications: A DFT study, *Physica B: Condensed Matter* **646** (2022) 414305.

3. Yuan, *et al.* - Pressure-engineered optical properties and emergent superconductivity in chalcopyrite semiconductor ZnSiP₂, NPG Asia Materials **13** (15) (2021).
4. J. L. Shay, J. H. Wernick - Ternary Chalcopyrite Semiconductors: Growth, Electronic Properties and Applications, Pergamon Press, New York, 1975.
5. I. Vurgaftman, J. R. Mayer, L. R. Ram Mohan - Band parameters for III–V compound semiconductors and their alloys, J. Appl. Phys. **89** (11) (2001) 5815-5875.
6. R. R. Reddy, K. R. Gopal, K. Narasimhullu, *et al.* - Correlation between optical electronegativity and refractive index of ternary chalcopyrites, semiconductors, insulators, oxides and alkali halides, Opt. Mater. **31** (2008) 209-212.
7. R. S. Indolia - Relationship of refractive index with optical energy gap and average energy gap for II-VI and III-V group of semiconductors, Int. J. Pure Appl. Phys. **13** (2) (2017) 185-191.
8. H. M. Gomaa, I. S. Yahia, H. Y. Zahran - Correlation between the static refractive index and the optical bandgap: Review and new empirical approach, Physica B: Condensed Matter **620** (2021) 413246.
9. V. Kumar, S. K. Tripathy, V. Jha - Second order nonlinear optical properties of A^IB^{III}C₂^{VI} chalcopyrite semiconductors, Appl. Phys. Lett. **101** (2012) 192105 (1-5).
10. V. Kumar, S. K. Tripathy, V. Jha, B. P. Singh - Second-harmonic generation properties of A^{II}B^{IV}C₂^V chalcopyrite semiconductors, Phys. Lett. A **378** (2014) 519-523.
11. T. S. Moss - A relationship between the refractive index and the infra-red threshold of sensitivity for photoconductors, Proc. Phys. Soc. B **63** (1950) 167.
12. T. S. Moss - Photoconductivity in Elements, Butterworth London, 1952, p. 61.
13. T. S. Moss - Relations between the refractive index and energy gap of semiconductors, Phys. Stat. Sol. B **131** (1985) 415-427.
14. A. Kumar, N. M. Ravindra, R. Rath - Optoelectronic properties of alkali halides, J. Phys. Chem. Sol. **40** (1979) 1141-1142.
15. N. M. Ravindra, S. Auluck, V. K. Srivastava - On the Pen gap in semiconductors, Phys. Stat. Sol. B **93** (1979) K155-K160.
16. V. P. Gupta, N. M. Ravindra - Comments on the Moss formula, Phys. Stat. Sol. B **100** (1980) 715-719.
17. N. M. Ravindra, V. K. Srivastava - Variation of refractive index with energy gap in semiconductors, Infrared Phys. **19** (1979) 603-604.
18. P. J. L. Herve, L. K. J. Vandamme - General relation between refractive index and energy gap in semiconductors, Infrared Phys. **35** (4) (1994) 609-615.
19. M. Anani, C. Malhieu, S. Lebid, Y. Amar, Z. Chama, H. Abid - Model for calculating the refractive index of a III-V semiconductor, Comput. Mater. Sci. **41** (2008) 570-575.
20. V. Kumar, J. K. Singh - Model for calculating the refractive index of different materials, Ind. J. Pure and Appl. Phys. **48** (2010) 571-574.
21. S. K. Tripathi - Refractive indices of semiconductors from energy gaps, Opt. Matter **46** (2015) 240-246.

22. V. Kumar, A. Sinha, B. P. Singh, A. P. Sinha, V. Jha - Refractive index and electronic polarizability of ternary chalcopyrite semiconductors, *Chin. Phys. Lett.* **32** (2015) 127701(1-5).
23. S. Ahmad, M. Ashraf, A. Ahmad, D. V. Singh - Electronic and optical properties of semiconductors and alkali halides, *Arab J. Sci. Engg.* **38** (2013) 1889-1894.
24. S. Ahmad, M. M. Haq - A study of energy gap, refractive index and electronic polarizability of ternary chalcopyrite semiconductors, *Iran. J. Phys. Res.* **14** (3) (2014) 89-93.
25. A. Bahadur, P. Mishra - Correlation between refractive index and electronegativity difference for $A^N B^{8-N}$ type binary semiconductors, *Acta Phys. Polo. A* **123** (4) (2013) 737-740.
26. CRC Handbook of Optical Materials, Marvin J. Weber (Ed.), 2003, pp. 62-75.
27. P. Ranjan, P. Kumar, P. K. Surolia, T. Chakraborty - Structure, electronic and optical properties of chalcopyrite semiconductor $AgTiX_2$ ($X = S, Se, Te$): A density functional theory study, *Thin Solid Films* **717** (1) (2021) 138469.