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Refractive Index and Electronic Polarizability of Ternary Chalcopyrite Semiconductors

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Simple models are proposed for the calculation of refractive index n and electronic polarizability α of $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ groups of chalcopyrite semiconductors from their energy gap data. The values of n and α for 2 compounds of $A^{I}B^{III}C_2^{VI}$ family and 12 compounds of $A^{II}B^{IV}C_2^{V}$ family are calculated for the first time in this work. The proposed models are applicable for the whole range of energy gap materials. The calculated values are compared with the available experimental and reported values. A fairly good agreement between them is obtained.

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The chalcopyrite structure is essentially a superlattice of the zincblende structure obtained by doubling its unit cube along the z-axis that becomes the c-axis of the chalcopyrite structure. The $A^{I}B^{III}C_2^{VI}$ group of chalcopyrites are analogous to II–VI compounds and can be obtained by replacing the group-II element alternatively by group-I and group-III elements. However, $A^{II}B^{IV}C_2^{V}$ chalcopyrites are similar to III–V compounds which can be obtained by replacing the group-III element alternatively by group-II and group-IV elements. New chalcopyrites of the $A^{II}B^{IV}C_2^{V}$ family have been recently developed by substituting A^{II}-type atoms with Be, Mn and Mg atoms,[1,2] which are less studied. The $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ semiconductors have potential applications in various linear and nonlinear optical devices.[3–5] In view of the above potential applications, the study of refractive index n and electronic polarizability α has recently become more interesting. Various theoretical models have been proposed for the calculations of the numerical values of n[6–14] and α[15–25] by different researchers. The models proposed by earlier researchers have been widely used in different crystal structures but for limited energy gap materials. Some models are good for low energy gap materials and some for high energy gap materials, while none of them are precisely applicable for the whole range of energy gap materials. Most of the earlier models are complex in nature and require a number of experimental data in their calculations, which are unknown for some of $A^{I}B^{III}C_2^{VI}$ compounds and the new magnetic materials of $A^{II}B^{IV}C_2^{V}$ family. Therefore, it would be of great interest to develop simple models for the calculation of n and α, which can be applicable for the whole range of energy gap materials. In this Letter, we propose two relations for the calculation of n and α, which are applicable for all compounds of these families including 2 new compounds of $A^{I}B^{III}C_2^{VI}$ group and 12 compounds of $A^{II}B^{IV}C_2^{V}$ group. The calculated values of n and α are in good agreement with the available experimental data and the calculated values reported.

Moss[6] has first proposed a relation $n = (K/E_g)^{1/4}$ for the calculation of refractive index n for a special class of semiconductors, where E_g is the energy gap of a semiconductor, and K is the constant equal to 95 eV. Later, Ravindra *et al.*[8] have modified the Moss relation and proposed a relation, $n = 4.084 + \beta E_g$, for low and high energy gap materials, where the constant $\beta = -0.62\,\text{eV}^{-1}$. This relation gives $n = 0$ if $E_g = 6.587$, which shows that the materials with $n \geq 4.084$ do not exist. However, there exist a number of materials such as GeTe, InSb, PbSe and PbTe having $n \geq 4.084$. The shortcomings of this relation have been discussed in detail by Finkernath.[26] Herve *et al.*[13] have used the oscillatory theory originally suggested by Penn[21] based on the random phase approximation for the dielectric function and proposed the following relation for the calculations of the refractive index,

$$n = \sqrt{1 + \left[\frac{A}{E_g + B}\right]^2}, \tag{1}$$

where A and B are the constants and equal to 13.6 and 3.4 eV, respectively. Equation (1) does not hold good for high energy gap materials.[27] Reddy *et al.*[28] have proposed the following relation between n and E_g by adding another arbitrary constant,

$$n = \sqrt{\frac{12.417}{[E_g - 0.365]^{1/2}}}, \tag{2}$$

which gives better results than the previous model[13] but cannot be used for low energy gap materials. The refractive index of $A^{III}B^{V}$ group of semiconductors, which are analogous to $A^{II}B^{IV}C_2^{V}$ semiconductors, has been correlated with E_g by Anani *et al.*[12] as $n^4 = 1 + C/E_g^2$, where C is a constant and equals to 40.8 eV.[12] This equation has been proposed by considering the fact that the refractive index for an infinite energy gap material is equal to one. The calculated values of n from this relation[12] have been found to be higher than the experimental values in both low and high energy gap materials. The details are given elsewhere[27] and will not be discussed here.

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Duffy[29] has correlated the energy gap with electronegativity by the relation $E_g = 3.72(\Delta\chi)$ for binary semiconductors. Based on this and Eq. (1), Reddy *et al.*[11] have further proposed the following relation between n and $\Delta\chi$,

$$n = \sqrt{1 + \left[\frac{D}{3.72\Delta\chi + E}\right]^2}, \tag{3}$$

where $\Delta\chi = [\chi_{\text{anion}} - \chi_{\text{cation}}]$ with χ_{anion} and χ_{cation} being the optical electronegativities of anion and cation, respectively, and D and E are constants. Equation (3) gives relatively better results for a low value of n (n = 1–2) but shows substantial deviation for high n (n=4–6) materials. Bahadur *et al.*[14] have also proposed a relation between n and $\Delta\chi$ as $n = F\Delta\chi^{-0.32}$, where F is the constant having different values for I–VII, II–VI, III–V and IV–VI groups of semiconductors. Recently, Kumar *et al.*[27] have proposed a simple relation $n = 3.3668(E_g)^{-0.32234}$ for the calculation of the refractive index of II–VI and III–V binary semiconductors, which is applicable for the entire range of energy gap materials. In this work, we propose the following relation based on the best fit of the data for the calculation of the refractive index of $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ groups of ternary chalcopyrites,

$$n = K_1 e^{-K_2 E_g}, \tag{4}$$

where K_1 and K_2 are constants. The numerical values of these constants have been obtained by simulating the known values of n and E_g of $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ chalcopyrites by using MATLAB software, and found to be 3.892 and 0.16, respectively, for K_1 and K_2. These values of constants are optimized with the experimental values of n and α. Equation (4) is applicable for all compounds of $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ families having the energy gap range 0.26 eV ($CdSnAs_2$)[30] to 3.50 eV ($CuAlS_2$)[31] including some new compounds. The calculated values of n are listed in Tables 1 and 2 along with the available experimental and reported values.

Electronic polarizability has been studied by several researchers.[32–34] Kumar *et al.*[32] have proposed the following relation for the calculations of total electronic polarizability of $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ chalcopyrites, based on Chemla,[18]

$$\begin{aligned}\alpha_{\text{tot}} &= (\alpha_{\text{AC}} + \alpha_{\text{BC}}) \\ &= (2a_0)^3 E_0^2 \left[\frac{D(\text{AC})}{E_{g,\text{AC}}^2} + \frac{D(\text{BC})}{E_{g,\text{BC}}^2}\right],\end{aligned} \tag{5}$$

where $a_0 = \hbar/me^2$, $E_0 = me^4/2\hbar^2$, α_{AC} and α_{BC} are the average polarizability of A–C and B–C bonds in ABC_2 compounds, m and e are the mass and charge of the electron, respectively, D(AC) and D(BC) are the correction factor for A–C and B–C bonds introduced by Vechen[16] to take into account the contribution of core electrons. Electronic polarizability of these chalcopyrites have also been calculated by using plasmon energy data and a well known relation given by Clausius,[33]

$$\alpha_{\text{CM}} = \frac{3}{4\pi N}\frac{(\varepsilon_{\text{av}} - 1)}{(\varepsilon_{\text{av}} + 2)}, \tag{6}$$

where N is the number of unit cells per cm^3 and ε_{av} is the average dielectric constant, i.e., $\varepsilon_{\text{av}}(ABC_2) = (\varepsilon_{\text{AC}} + \varepsilon_{\text{BC}})/2$, $\varepsilon_{\text{AC}} = 1 + (\hbar\omega_{\text{p,AC}}/E_{\text{g,AC}})^2$ and $\varepsilon_{\text{BC}} = 1 + (\hbar\omega_{\text{p,BC}}/E_{\text{g,BC}})^2$.

The relationship of the electronic polarizability α with bulk modulus B, molecular weight M and density σ has been proposed by Reddy *et al.*[34] for binary and ternary semiconductors,[22,34]

$$\alpha = 0.395 \times 10^{-24}\left[\frac{(5.563 - 0.033B)^2 - 1}{(5.563 - 0.033B)^2 + 2}\right]\frac{(M)}{(\sigma)}\ \text{cm}^3. \tag{7}$$

Recently, Verma *et al.*[25] have correlated α with the electronic and optical properties of solids and proposed the relations $\alpha = K'(V_X V_Y)^{0.45} d^3$ for binary zincblende crystals and $\alpha = K'(V_X V_Y V_Z)^{0.205} d^3$ for ABC_2 ternary chalcopyrites, where V_X, V_Y and V_Z are the numbers of valence electrons of atoms A, B and C, respectively, d is the nearest neighbor distance in Å and K' is the constant depending on the crystal structure. The values of K' are 0.142 and 0.55, respectively, for the zincblende and chalcopyrite semiconductors. In this work, we propose the following simple relation for the calculation of the electronic polarizability of $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ groups of chalcopyrite semiconductors,

$$\alpha = K_3 (E_g)^{-K_4}, \tag{8}$$

where K_3 and K_4 are constants, which are obtained by simulating the known values of α and E_g by using simulation software. The numerical values of K_3 and K_4 are 20.050 and 0.4437, respectively, for $A^{I}B^{III}C_2^{VI}$ compounds, and 17.320 and 0.1496 for $A^{II}B^{IV}C_2^{V}$ compounds. The calculated values of α from Eq. (8) are listed in Tables 1 and 2.

By using Eqs. (4) and (8), the values of n and α of $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ groups of chalcopyrites have been calculated, as listed in Table 1 along with the available experimental and reported values.[35–37] A fairly good agreement between them has been obtained. Table 1 shows that our calculated values are more close to the experimental values than the values reported by earlier researchers. This shows that our exponential fit is more preferable than the fit with other functions, which gives the physical explanation of proposed Eqs. (4) and (8). The values of n and for 2 new compounds of $A^{I}B^{III}C_2^{VI}$ family and 12 new compounds of $A^{II}B^{IV}C_2^{V}$ family have been calculated for the first time in this work and listed in the bottom rows of Table 1. The experimental values of these 14 compounds are not available for comparison and await experimental verification. The predictive nature of Eqs. (4) and (8) are of great importance in predicting the values of n and of new compounds of these families. The validity of Eq. (4) has also been tested for some of defect chalcopyrites of $A^{II}B_2^{IV}C_4^{V}$ family[38] for which the experimental values of E_g are

known. Surprisingly, a good agreement has been obtained between the calculated and reported values of n. For example, the experimental values of E_g for $ZnIn_2Te_4$, $CdGa_2S_4$, $CdGa_2Te_4$, $HgGa_2S_4$, and $HgGa_2Se_4$ defect chalcopyrites are 1.87 eV, 3.25 eV, 1.50 eV, 2.79 eV and 1.95 eV,[39] respectively. By using Eq. (4), the calculated values of n for these defect chalcopyrites have been found to be 2.88, 2.31, 3.06, 2.49 and 2.84, respectively, against the reported values 2.73,[40] 2.37,[41] 3.38,[42] 2.55[43] and 2.77,[43] which are in good agreement. The main advantage of the present models is the simplicity of the formulas, which do not require any experimental data except the energy gap, while the earlier models require the experimental values of parameters such as molecular weight, electronegativity, plasmon energy, dielectric constant, bulk modulus and density in their calculations.

Table 1. Refractive index n of $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ chalcopyrite semiconductors.

Compounds		n					
				Reported			
$A^{I}B^{III}C_2^{VI}$	Known E_g (eV)	Expt[6,44,45]	Calc (Eq. (4))	Herve *et al.*[13]	Moss[61]	Ravindra *et al.*[46]	Reddy *et al.*[47]
$CuAlS_2$	3.50*[30]	2.40	2.22		2.28	1.91	2.33
$CuAlSe_2$	2.70,*[30] 2.65,[49] 2.71[50]	2.60	2.52	2.45	2.44	2.41	2.59
$CuAlTe_2$	2.06,[30] 0.88*[48]	3.30	2.79	2.69	2.61	3.52	3.69
$CuGaS_2$	2.40,[30] 2.43,*[49] 2.5[50]	2.67	2.63	2.55	2.51	2.53	2.71
$CuGaSe_2$	1.70,[30] 1.68,[49] 1.59,[51] 1.73,[52] 2.03,[53] 2.11*[3]	2.80	2.77	2.85	2.74	3.03	3.06
$CuGaTe_2$	1,*[30] 1.23,[50] 1.89[54]	3.30	3.31	3.25	3.12	3.46	3.59
$CuInS_2$	1.50,[30] 1.48,[54] 1.53,[3] 1.55*[53]	2.60	3.03		2.82	3.15	3.18
$CuInSe_2$	1.04,*[3] 1,[50] 0.88,[55] 0.96,[56] 0.98,[53] 1.01[57]	2.90	3.16		3.15	3.49	3.63
$CuInTe_2$	0.96,*[30] 1–1.15,[50] 1.06[3]	3.40	3.34	3.29	3.16	3.49	3.64
$AgAlS_2$	3.13*[30]	2.30	2.35	2.31	2.35	2.15	2.45
$AgAlSe_2$	2.55*[30]	2.47	2.58	2.50	2.47	2.50	2.66
$AgAlTe_2$	2.27,*[30] 2.2[50]	2.54	2.70	2.60	2.55	2.68	2.77
$AgGaS_2$	2.70,[30] 2.55,[50] 2.72,*[57] 2.64,[3] 2.43[58]	2.40	2.51	2.45	2.44	2.41	2.59
$AgGaSe_2$	1.80,[3] 1.83,*[57] 1.76[58]	2.80	2.90	2.80	2.70	2.96	3.00
$AgGaTe_2$	1.10,[30] 1.1–1.3,[50] 1.21,*[48] 1.32,[3] 1.36[53]	3.30	3.20	3.19	3.05	3.40	3.49
$AgInS_2$	2.0,[30] 1.87*[49]	2.50	2.88		2.63	2.84	2.89
$AgInSe_2$	1.24,[30] 0.96*[49]	3.32	3.19	3.10	2.96	3.31	
$AgInTe_2$	1*[30]	3.40	3.30	3.25	3.12	3.46	3.66
$CuFeS_2$	1.07[48]		3.27				
$CuFeSe_2$	0.53[48]		3.57				
$A^{II}B^{IV}C_2^{V}$							
$ZnSiP_2$	2.1,*[30] 2.3,[48] 2.96[50]	3.10	2.78		2.6	2.78	2.84
$ZnGeP_2$	1.99,*[30] 2.2,[48] 2.34[50]	3.10	2.83	2.67	2.63	2.85	2.90
$ZnSnP_2$	1.66,*[30,49] 1.45[48]	2.90	2.98	2.72	2.75	3.06	3.10
$CdSiP_2$	2.45,*[30] 2.2[48]	3.10	2.73	2.87	2.50	2.56	2.80
$CdGeP_2$	1.72,*[30] 1.8[48]	3.30	2.95	2.53	2.73	3.02	3.40
$CdSnP_2$	1.17,*[30] 1.5[48]	3.10	3.22	2.84	3.01	3.36	3.43
$ZnSiAs_2$	1.70,*[30] 2.1[50]	3.10	2.96	3.14	2.74	3.03	3.06
$ZnGeAs_2$	1.15,*[30] 0.85[48]	3.50	3.23	2.85	3.02	3.37	3.75
$ZnSnAs_2$	0.73,*[30] 0.65[48]	3.60	3.46	3.15	3.48	3.68	4.02
$CdSiAs_2$	1.55,*[30] 1.6[48]	3.50	3.50		2.80	3.12	3.15
$CdGeAs_2$	0.57,*[30] 0.53[48]	3.40	3.55	2.93	3.53	3.7	4.08
$CdSnAs_2$	0.26[30]	3.70	3.73		4.37	3.92	4.93
$BeSiAs_2$	1.1[59]		3.26				
$BeGeP_2$	0.9[59]		3.37				
$BeGeAs_2$	1.68[51]		2.97				
$BeSnP_2$	1.98[51]		2.83				
$BeSnAs_2$	1.15[51]		3.23				
$MgSiP_2$	2.0,*[1] 2.26[1]		2.82				
$MgSiAs_2$	2.67,[51] 2.0,*[52] 2.08[60]		2.82				
$MgGeP_2$	3.0,[51] 2.17,[52] 2.1*[60]		2.78				
$MgGeAs_2$	2.18,[51] 1.6*[52,60]		3.01				
$MgSnP_2$	2.48,[51] 1.8,[52] 1.56*[60]		3.03				
$MgSnAs_2$	1.2,[52] 0.93,*[60] 1.65[51]		3.35				
$MnGeP_2$	0.24[57]		3.74				

Table 2. Electronic polarizability α of $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ chalcopyrite semiconductors.

Compounds	$\alpha\,(10^{-24})\,\mathrm{cm}^3$							
	Known (CM)[6,48]	This work	Reported					
$A^{I}B^{III}C_2^{VI}$		Eq. (8)	Kumar *et al.*[32]	Gupta *et al.*[31]	Reddy *et al.*		Li *et al.*[43]	Verma *et al.*[25]
					Ref. [28]	Ref. [22]		
$CuAlS_2$	10.79	11.55	6.62	6.73	11.74	10.84	6.40	11.95
$CuAlSe_2$	13.72	12.95	9.02	10.09	14.70	14.48	10.00	13.75
$CuAlTe_2$	19.05	21.21	7.37	17.17	18.38	18.31	17.00	17.08
$CuGaS_2$	12.03	13.56	7.61	7.25	12.90	12.27	7.20	12.10
$CuGaSe_2$	14.38	14.43	10.29	10.91	15.82	15.73	11.00	14.10
$CuGaTe_2$	19.65	20.05	11.74	19.2	21.25	20.09	19.00	17.48
$CuInS_2$	13.25	16.53	10.59	8.42	15.74	15.50	8.40	13.75
$CuInSe_2$	16.38	19.70	12.73	12.47	18.99	18.26	13.00	15.73
$CuInTe_2$	21.86	20.41	15.29	20.86	23.46	22.39	21.00	19.15
$AgAlS_2$	11.94	12.13	7.78	9.02	13.63		7.50	13.75
$AgAlSe_2$	14.36	13.28	10.42	11.31	16.23	16.03	12.00	15.73
$AgAlTe_2$	16.08	13.97	12.06	19.35	18.13	18.03	19.00	19.15
$AgGaS_2$	12.4	12.90	8.46	8.22	14.24	14.14	8.30	14.10
$AgGaSe_2$	15.77	15.36	11.35	12.13	17.19	17.06	13.00	16.11
$AgGaTe_2$	21.68	18.43	13.17	20.79	23.12	22.05	21.00	19.36
$AgInS_2$	14.42	15.22	10.91	9.04	16.86	17.08	9.50	15.36
$AgInSe_2$	19.91	20.41	14.69	13.51	20.80	20.28	14.00	17.69
$AgInTe_2$	24.02	20.05	16.88	23.23	25.59	22.98	23.00	21.37
$CuFeS_2$		19.46						
$CuFeSe_2$		26.51						
$A^{II}B^{IV}C_2^{V}$								
$ZnSiP_2$	13.42	15.61	10.70	12.45	13.35	12.12	12.00	14.44
$ZnGeP_2$	14.04	15.72	11.28	14.24	14.10	13.60	14.00	15.21
$ZnSnP_2$	21.85	16.13	13.80	16.36		23.38	16.00	17.23
$CdSiP_2$	14.82	15.27	12.29	14.34	14.34	14.40	14.00	16.20
$CdGeP_2$	16.70	16.05	12.88	15.95	16.62	16.51	16.00	17.02
$CdSnP_2$	15.58	16.94	17.65	18.40			19.00	19.20
$ZnSiAs_2$	15.09	16.07	12.89	18.12	15.57	0.93	19.00	16.40
$ZnGeAs_2$	16.86	16.98	12.62	20.52	17.37	16.84	21.00	17.02
$ZnSnAs_2$		18.10	14.99	23.84	20.68	19.24	23.00	18.97
$CdSiAs_2$	16.37	16.28	13.72	20.71			21.00	18.09
$CdGeAs_2$	18.39	18.73	12.15	23.16	21.22	19.21	23.00	18.97
$CdSnAs_2$	21.27	20.91	17.32	26.68		21.71	26.00	21.07
$BeSiAs_2$		17.09						
$BeGeP_2$		17.57						
$BeGeAs_2$		16.10						
$BeSnP_2$		15.74						
$BeSnAs_2$		16.98						
$MgSiP_2$		15.71						
$MgSiAs_2$		15.71						
$MgGeP_2$		15.61						
$MgGeAs_2$		16.21						
$MgSnP_2$		16.27						
$MgSnAs_2$		17.49						
$MnGeP_2$		21.15						

*These experimental values of E_g in Tables 1 and 2 have been taken for simulating the values of constants K_1–K_4 in Eqs. (4) and (8).

In almost all cases, our calculated values of n and α from the proposed models are closer to the experimental data than the models proposed by earlier researchers. Thus one can predict the values of n and α of new compounds of $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ families from their energy gap data.

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