Empirical temperature dependence of the refractive index of semiconductors

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Values of the temperature coefficient of the refractive index were obtained from the derivation of a simple relation between energy band-gap and refractive index in semiconductors. These values, $(dn/dT)/n$, were compared to the experimental data found in literature. Our model, with only one fitting parameter $dB/dT=2.5\times10^{-5}$ K^{-1} for all semiconductors, results in the best agreement with experimental data. © *1995 American Institute of Physics.*

Sometimes, it is useful to have a rule of thumb[1] or an empirical relation, for the mobility,[2] for example, to make a first estimation in modelling devices. 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. Our aim is to show how these expressions give good approximations for the temperature coefficient of the refractive index for several semiconductors. For that reason, we used experimentally observed data.[6-10] The experimental results were measured far from the absorption edge. The temperature dependence of the energy band gap E_G (eV) is denoted by dE_G/dT (eV K^{-1}), the temperature coefficient for the refractive index by $(dn/dT)/n$ (K^{-1}), and the temperature by T(K). From the empirical relations, we derived the temperature behavior. We compared the results obtained for a dozen of different semiconductors (IV, III-V, IV-VI). Our temperature-dependence relation results in the best agreement with experimental data.

Here, we will quickly review the various relations between n and E_G. Moss[3] presented the following equation, based on an atomic model:

$$n^4 E_G = K, \tag{1}$$

where the constant K is originally 95 eV and was found to be 108 eV by Ravindra et al.[11] Later on,[4] they gave a linear form of n as a function of E_G:

$$n = \alpha + \beta E_G \tag{2}$$

with $\alpha = 4.084$ and $\beta = -0.62$ eV^{-1}

Inspired by simple physics of light refraction and dispersion, where the dielectric function is

$$\epsilon(\omega) = 1 + \frac{Nq^2}{m\epsilon_0} \frac{1}{\omega_0^2 - \omega^2} \tag{3}$$

with ϵ_0 the permittivity of free space, N the density of valence electrons, m the rest mass of electrons, and ω_0 the ultraviolet resonance frequency, we proposed an empirical relation for $\omega \ll \omega_0$, as follows:[5]

$$n = \sqrt{1 + \left(\frac{A}{E_G + B}\right)^2} \tag{4}$$

with $A = 13.6$ eV and $B = 3.4$ eV, henceforth our model is denoted by HV.

In Eqs. (1), (2), and (4), the temperature dependence of n stems from the variation of E_G with T and from the constants involved in the relations. In order to check which temperature-dependence relation is the best, we assume the constants to be linear functions of T. In Eq. (1) we will assume that both K and E_G are temperature dependent. Thus

$$\frac{1}{n}\frac{dn_{\text{Moss}}}{dT} = \frac{1}{4}\left(\frac{K_1}{K} - \frac{1}{E_G}\frac{dE_G}{dT}\right) \quad \text{with} \quad K_1 = \frac{dK}{dT}. \tag{5}$$

In Eq. (2), two constants play a role, but we only considered the constant β (-0.62 eV^{-1} at 300 K) to be linearly temperature dependent. It results in

$$\frac{1}{n}\frac{dn_{\text{Ravindra}}}{dT} = \left(\beta_1 E_G + \frac{dE_G}{dT}\beta\right)\left(\frac{1}{\alpha + \beta T}\right)$$
$$\text{with} \quad \beta_1 = \frac{d\beta}{dT}. \tag{6}$$

In our Eq. (4), we have shown that the parameter B (3.4 eV) was a function of the incident-photon wavelength,[12] but this energy will be considered as a linear function of temperature. Hence, we find for the temperature coefficient of the refractive index

$$\frac{dn_{\text{HV}}}{dT} = -\frac{(13.6)^2}{n(E_G+B)^3}\left(\frac{dE_G}{dT} + B_1\right) \quad \text{with} \quad B_1 = \frac{dB}{dT}. \tag{7}$$

After substitution of the expression $E_G + B = [(13.6^2/n^2) - 1]^{1/2}$ in Eq. (7), we have

$$\frac{1}{n}\frac{dn_{\text{HV}}}{dT} = -\frac{(n^2-1)^{3/2}}{13.6n^2}\left(\frac{dE_G}{dT} + B_1\right). \tag{8}$$

The various semiconductors and data used are shown in Table I. The parameters K_1, β_1, or B_1, are constant for the all the materials studied. They were computed to result in the lowest deviation between experimental data and the values given by Eqs. (5), (6), and (8). They are found to be 6.68×10^{-4}, -5.15×10^{-6}, and 2.5×10^{-5} eV K^{-1}, respectively.

The temperature coefficient of the refractive indices of the various materials are plotted versus the energy band gap

TABLE I. Experimental values of the energy band gap and its temperature coefficient and the refractive index temperature-dependence for some semiconductors.

| Material	E_G (eV)	dE_G/dT (eV K^{-1})	$(dn/dT)/n$ (K^{-1})	Reference
InSb	0.18	-2.8×10^{-4}	6.9×10^{-5}	6
PbSe	0.278	$+5.1\times10^{-4}$	-2.1×10^{-4}	7
Ge	0.67	-3.7×10^{-4}	6.9×10^{-5}	8
GaSb	0.75	-3.7×10^{-4}	8.2×10^{-5}	6
Si	1.1	-2.8×10^{-4}	4.0×10^{-5}	8
InP	1.35	-2.9×10^{-4}	2.7×10^{-5}	6
GaAs	1.43	-3.9×10^{-4}	4.5×10^{-5}	6
AlAs	2.15	-4.0×10^{-4}	4.6×10^{-5}	9
AlP	2.41	-3.7×10^{-4}	3.6×10^{-5}	9
SiC	2.86	-3.3×10^{-4}	2.9×10^{-5}	6
GaN	3.5	-4.8×10^{-4}	2.6×10^{-5}	6
C	5.48	-5.0×10^{-5}	4.0×10^{-6}	10

FIG. 1. Plot of the temperature coefficient of the refractive index vs the energy band gap. The line stands for the experimental results. The crosses ($\times$) stand for Eq. (5), based on Moss' relation. The crosses (+) are for Eq. (6), based on the relation of Ravindra et al., and the open squares ($\square$) for our model HV [Eq. (8)].

in Fig. 1. The calculated values, given by Eqs. (5), (6), and (8) which are based on the relations of Moss, Ravindra et al., Hervé and Vandamme, respectively, are presented on the same graph.

Among some classical semiconductors, two show particular temperature dependences. Usually, when T increases, E_G decreases (the band-gap temperature coefficient is between -2×10^{-4} and -5×10^{-4} eV K^{-1}) and n increases (about a few 10^{-4} K^{-1}). Diamond presents a 5–10 times lower energy band-gap temperature dependence being -5×10^{-5} eV K^{-1}. Besides that, its refractive index temperature coefficient is about ten times lower than for other semiconductors presented (4×10^{-6} K^{-1}). Knowing the energy band gap and its temperature variation, the three relations are able to predict this particularly small value of the refractive index temperature coefficient (giving results between 2×10^{-6} and -4×10^{-6} K^{-1}).

The second semiconductor showing particular properties is the lead selenide. Like others from its group, dE_G/dT is positive and $(dn/dT)/n$ is negative. Equations (5), (6), and (8) are, again, able to give good estimations of that particular behaviour, however with a larger dispersion (-8×10^{-5} to -4.5×10^{-4} K^{-1}).

From Fig. 1, we see that all the relations are able to follow the trend of the experimental results. However, we observe that Moss' relation gives a strong deviation at low energy band gap (<1.43 eV). Above that value, this relation is the closest to the experiment results. On the other hand, Ravindra's relation provides more accurate estimations below 1.43 eV than Moss' one, and starts to deviate at higher energies (>1.43 eV). Compared to these two relations, our model Eq. (8) presents a better overall behaviour. It gives the best results below 1.43 eV, and it is quite close to the experimental values above that energy.
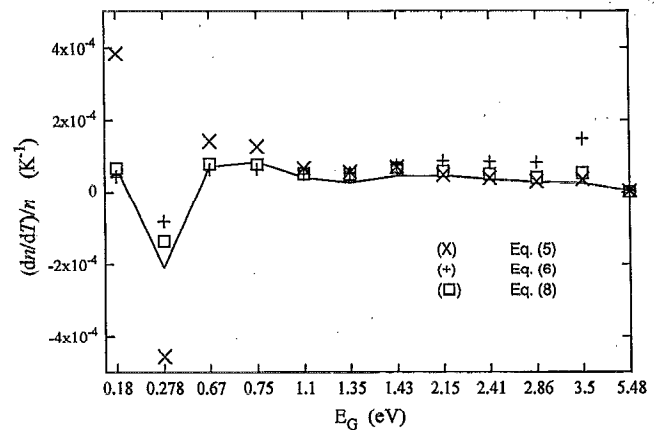
Three relations for the temperature dependence of the refractive index are proposed and compared for various semiconductors. From our empirical relation between energy band gap E_G and refractive index n [$n^2-1=A^2/(E_G+B)^2$, with $A=13.6$ and $B=3.4$ eV], we obtained overall good results for the temperature coefficient $(dn/dT)/n$. The trend of the predicted values are in good agreement with the experimental data, even for some semiconductors like C or PbSe that exhibit special behavior. Two parameters were considered to be temperature dependent: E_G the energy band gap and the coefficient $B_1=dB/dT=2.5\times10^{-5}$ K^{-1}. This coefficient is constant for all the materials studied and $(dn/dT)/n=-(n^2-1)^{3/2}(dE_G/dT+B_1)/(13.6n^2)$.

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