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:

\[ n^4E_G = K, \]  

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 \(E_G\):

\[ n = \alpha + \beta E_G \]  

with \(\alpha=4.084\) and \(\beta=-0.62\) eV\(^{-1}\).

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

\[ \varepsilon(\omega) = 1 + \frac{Nq^2}{m\varepsilon_0} \left( \frac{1}{\omega_0^2} - \omega^2 \right) \]  

with \(\varepsilon_0\) the permittivity of free space, \(N\) the density of valence electrons, \(m\) the rest mass of electrons, and \(\omega_0\) the ultraviolet resonance frequency, we proposed an empirical relation for \(n\) as a function of \(E_G\):

\[ n = \sqrt{1 + \left( \frac{A}{E_G + B} \right)^2} \]  

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

\[ \frac{1}{n} \frac{dn_{\text{Moss}}}{dT} = \frac{1}{4} \left( \frac{K_1}{K} \right) \frac{1}{E_G} \frac{dE_G}{dT} \]  

with \(K_1 = \frac{dK}{dT}\).

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

\[ \frac{1}{n} \frac{dn_{\text{Ravindra}}}{dT} = \left( \beta_1 E_G + \frac{dE_G}{dT} \right) \frac{1}{\alpha + \beta T} \]  

with \(\beta_1 = \frac{dB}{dT}\).

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

\[ \frac{dn_{\text{HV}}}{dT} = -\frac{(13.6)^2}{n(E_G+B)^3} \left( \frac{dE_G}{dT} + B_1 \right) \]  

with \(B_1 = \frac{dB}{dT}\).

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

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

The various semiconductors and data used are shown in Table I. The parameters \(K_1\), \(\beta_1\), 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\times10^{-4}, -5.15\times10^{-6}, and 2.5\times10^{-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.

<table>
<thead>
<tr>
<th>Material</th>
<th>( E_G ) (eV)</th>
<th>( \frac{dE_G}{dT} ) (eV K(^{-1}))</th>
<th>( \frac{dn}{dn} ) (K(^{-1}))</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>InSb</td>
<td>0.18</td>
<td>(-2.8 \times 10^{-4})</td>
<td>(6.9 \times 10^{-5})</td>
<td>6</td>
</tr>
<tr>
<td>InSe</td>
<td>0.279</td>
<td>(+5.1 \times 10^{-4})</td>
<td>(-2.1 \times 10^{-4})</td>
<td>7</td>
</tr>
<tr>
<td>Ge</td>
<td>0.67</td>
<td>(-3.7 \times 10^{-4})</td>
<td>(6.9 \times 10^{-5})</td>
<td>8</td>
</tr>
<tr>
<td>GaSb</td>
<td>0.75</td>
<td>(-3.7 \times 10^{-4})</td>
<td>(8.2 \times 10^{-5})</td>
<td>6</td>
</tr>
<tr>
<td>Si</td>
<td>1.1</td>
<td>(-2.8 \times 10^{-4})</td>
<td>(4.0 \times 10^{-3})</td>
<td>6</td>
</tr>
<tr>
<td>InP</td>
<td>1.35</td>
<td>(-2.9 \times 10^{-4})</td>
<td>(2.7 \times 10^{-5})</td>
<td>6</td>
</tr>
<tr>
<td>GaAs</td>
<td>1.43</td>
<td>(-3.9 \times 10^{-4})</td>
<td>(4.5 \times 10^{-5})</td>
<td>6</td>
</tr>
<tr>
<td>AlAs</td>
<td>2.15</td>
<td>(-4.0 \times 10^{-4})</td>
<td>(4.6 \times 10^{-5})</td>
<td>6</td>
</tr>
<tr>
<td>AlP</td>
<td>2.41</td>
<td>(-3.7 \times 10^{-4})</td>
<td>(3.6 \times 10^{-5})</td>
<td>9</td>
</tr>
<tr>
<td>SiC</td>
<td>2.96</td>
<td>(-2.3 \times 10^{-4})</td>
<td>(2.9 \times 10^{-5})</td>
<td>6</td>
</tr>
<tr>
<td>GaN</td>
<td>3.5</td>
<td>(-4.8 \times 10^{-4})</td>
<td>(2.6 \times 10^{-5})</td>
<td>6</td>
</tr>
<tr>
<td>C</td>
<td>5.48</td>
<td>(-5.0 \times 10^{-5})</td>
<td>(4.0 \times 10^{-6})</td>
<td>10</td>
</tr>
</tbody>
</table>

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 \(-2 \times 10^{-4}\) and \(-5 \times 10^{-4} \text{ eV K}^{-1}\)) and \( n \) increases (about a few \(10^{-4} \text{ K}^{-1}\)). Diamond presents a 5–10 times lower energy band-gap temperature dependence being \(-5 \times 10^{-5} \text{ eV K}^{-1}\). Besides that, its refractive index temperature coefficient is about ten times lower than for other semiconductors presented (\(4 \times 10^{-6} \text{ K}^{-1}\)). 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 \(2 \times 10^{-6}\) and \(-4 \times 10^{-6} \text{ K}^{-1}\)).

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 (\(-8 \times 10^{-5}\) to \(-4.5 \times 10^{-5} \text{ K}^{-1}\)).

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 behavior. 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 \( B=3.4 \text{ eV} \), 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 \( B_1=dB/dT=2.5 \times 10^{-5} \text{ K}^{-1} \). This coefficient is constant for all the materials studied and \( (dn/dT)/n=-\left(n^2-1\right)^{3/2}(dE_G/dT+B_1)/(13.6n^2) \).