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Empirical temperature dependence of the refractive index of semiconductors

P. J. L. Hervé and L. K. J. Vandamme
Department of Electrical Engineering, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

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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, \( \frac{dn}{dT} \), were compared to the experimental data found in literature. Our model, with only one fitting parameter \( \frac{dB}{dT} = 2.5 \times 10^{-5} \text{ K}^{-1} \) 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 or an empirical relation, for the mobility, for example, to make a first estimation in modelling devices. A few empirical relations 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.

The experimental results were measured far from the absorption edge. The temperature dependence of the energy band gap \( E_G (\text{eV}) \) is denoted by \( \frac{dE_G}{dT} (\text{eV K}^{-1}) \), the temperature coefficient for the refractive index by \( \frac{dn}{dT} (\text{K}^{-1}) \), and the temperature by \( T (\text{K}) \). 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 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. Later on, 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 \( \beta = -0.62 \text{ eV}^{-1} \).

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

\[
e(\omega) = 1 + \frac{Nq^2}{m e_0^2} \frac{1}{\omega_0^2 - \omega^2} \tag{3}
\]

with \( e_0 \) 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 \( \omega \ll \omega_0 \), as follows:

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

with \( A = 13.6 \text{ eV} \) and \( B = 3.4 \text{ eV} \), 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

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

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

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

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

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

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 \( K_1 \), \( \beta_1 \), or \( B_1 \), are constant for 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 \( 6.68 \times 10^{-4} \), \( -5.15 \times 10^{-6} \), and \( 2.5 \times 10^{-5} \text{ eV} \text{ K}^{-1} \), 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/dT)ln}{(K^{-1})} )</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>InSb</td>
<td>0.18</td>
<td>(-2.8\times10^{-4})</td>
<td>(6.9\times10^{-3})</td>
<td>6</td>
</tr>
</tbody>
</table>
| P
| 0.278 | +5.1\times10^{-4} | 2.1\times10^{-4} | 7 |
| Ge       | 0.67           | \(-3.7\times10^{-4}\) | \(6.9\times10^{-5}\) | 8         |
| GaSb     | 0.75           | \(-3.7\times10^{-4}\) | \(8.2\times10^{-5}\) | 6         |
| Si       | 1.1            | \(-2.8\times10^{-4}\) | \(4.0\times10^{-3}\) | 8         |
| InP      | 1.35           | \(-2.9\times10^{-4}\) | \(2.7\times10^{-5}\) | 6         |
| GaAs     | 1.43           | \(-3.9\times10^{-4}\) | \(4.5\times10^{-5}\) | 6         |
| AlAs     | 2.15           | \(-4.0\times10^{-4}\) | \(4.6\times10^{-5}\) | 9         |
| AlP      | 2.41           | \(-3.7\times10^{-4}\) | \(3.6\times10^{-5}\) | 9         |
| SiC      | 2.96           | \(3.3\times10^{-4}\)  | \(2.9\times10^{-5}\) | 6         |
| GaN      | 3.5            | \(-4.8\times10^{-4}\) | \(2.6\times10^{-5}\) | 6         |
| C        | 5.48           | \(-5.0\times10^{-5}\) | \(4.0\times10^{-6}\) | 10        |

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 \( n \) \( n^2 - 1 = A(E_G + B)^2 \), with \( A = 13.6 \) and \( B = 3.4 \) eV, we obtained overall good results for the temperature coefficient \( (dn/dT)ln \). 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 \( (dn/dT)ln = -(n^2 - 1)^{3/2}(dE_G/dT + B_1)(13.6n^2)^2 \).