To Study the dependency of linear thermal expansion coefficient and Melting Temperature on Plasmon energy in case of II-VI and III-V groups of binary semiconductors

R.S. Indolia

Dept. Of Physics, Agra College, Agra, India.

Abstract

Linear Thermal expansion coefficient ($\alpha_L$), Melting temperature ($T_m$) of II-VI and III-V groups of binary semiconductors have been calculated by using Plasmon energy data. On the basis of linear plots, a new relation has been developed between melting temperature and Plasmon energy, by using this developed equation a new empirical relation between linear thermal expansion coefficient and Plasmon energy has been developed for II-VI and III-V groups of binary semiconductors. The calculated values of $\alpha_L$ and $T_m$ by using developed equations are in close agreement with experimental and calculated values of different researchers.

Keywords: Linear thermal expansion coefficient, melting temperature, bond length, bond ionicity, Plasmon energy, II-VI and III-V groups of binary semiconductors.

INTRODUCTION:

Binary and Ternary semiconductors have obtained considerable importance because of their potential application in the areas of light emitting diodes, non-linear optics, photo-voltaic devices and solar cells [1-3]. The solid solutions of these
semiconductors have been used in electro-optic devices[3-5]. Their mixed
 crystals are being used for the fabrication of detectors, lasers and integrated optic
devices such as switches, modulators, filters, and for infrared generation [6-10].
Experimental methods used for calculating these parameters of binary and
ternary semiconductors are tedious, in the sense of their cost, and difficulties of
getting accurate values of some of methods. Therefore in the recent past, a
number of theoretical calculations based on empirical relations have become an
essential part of material research. In modern high speed computer techniques
empirical methods allow researchers to investigate many structural and physical
properties of materials only by computation or simulation instead of traditional
experiments. In many cases empirical relations do not give highly accurate
results for each specific material, but they still can be very useful. Empirical
concepts such as, ionicity and plasmon energy are than useful [11-13]. These
concepts are directly associated with the character of the chemical bond and thus
provide means for explaining and classifying many basic properties of binary
and ternary semiconductors.
Neuman[14] ,Kumar et al[15]have proposed relation between $\alpha_L$ and Plasmon
energy for binary tetrahedral semiconductors, Omar[16] proposed relationship
between $\alpha$ and bond length, Kumar[17]have shown that $T_m$ and Plasmon energy
of ternary semiconductors is linearly related, because both binary and ternary
semiconductors have tetrahedral structure therefore $T_m$ and Plasmon energy must
have some dependency with each other in case of binary semiconductors and an
empirical relation between $\alpha$ and Plasmon energy has been proposed for binary
semiconductors.

**THEORY:**
Using the theory proposed by Neumann [14], Kumar et al [15] have proposed an
expressions for linear thermal expansion coefficient $\alpha_L$ in terms of plasmon energy
$\hbar \omega_p$ for binary tetrahedral semiconductors, as follows :

$$\alpha_L = \frac{0.021}{T_m} - C \left[ d - d_o \right]^3$$  \hspace{1cm} (1)

The relationship between bond length and plasmon energy for II-VI and III-V
semiconductors by Kumar [15]

$$d = 15.30 \left( \hbar \omega_p \right)^{2/3}$$  \hspace{1cm} (2)

Where $d$ is in $\AA$ and $\hbar \omega_p$ in $eV$. 
by using equation 2

\[ \alpha_L = \frac{0.021}{T_m} - C \left[ 15.30 \left( h\nu_p \right)^{2/3} - d_o \right] \]  

(3)

where C is constant for a particular group of semiconductors, \( d_o \) is the bond length for diamond i.e. \( d_o = 1.545 \text{ Å} \), and \( T_m \) is the melting temperature. The values of \( C = 3.3 \) and \( 10.0 \left( 10^{-6} \text{ K}^{-1} \text{ Å}^{0.3} \right) \), and \( d_o = 1.382 \) and \( 1.561 \text{ Å} \) for II-VI and III-V semiconductor, are obtained by Neumann [14].

Recently Omar [16] has proposed the following equation, similar to equation (1) with some modification.

\[ \alpha_L = \frac{0.021}{T_m} - \left[ D(d - d_o) \right]\]  

(4)

where D is the slope of \( \Delta^{1/3} \) versus bond length plot, and the term is \( \Delta \) is the difference between the expected \( \alpha_L \) calculated for diamond which is equal to \( 0.021/T_m \) and that obtained by the measurement in the saturation region \( \alpha_L \).

Neumann [14] has proposed an approximate empirical relation between D and bond ionicity \( f_i \), and Omar [16] modified it in the form given as

\[ D^3 = b_0 - b_1 f_i^2 \]  

(5)

where \( b_0 \) and \( b_1 \) are constants having values 17.061 and \( 29.86 \times 10^{-6} \text{ K}^{-1} \text{ Å}^{0.3} \), respectively.

It is clear from equations (3) and (4) that these equations require experimental data of melting temperature of semiconductors, in their calculations. Recently Kumar et al. [17] have shown that in case of ternary semiconductors melting temperature is linearly related with plasmon energy[18]. Therefore we thought that it should also be applicable in case of binary semiconductors, because both have tetrahedral structure as discussed in previous chapter VIII. For this purpose we have plotted \( ln T_m \) versus \( ln h\nu_p \) in figure 1 for II-VI and III-V semiconductors. It is observed from the figure that all the data points can be fitted linearly. On the basis of this linear plot the relationship between \( T_m \) and \( h\nu_p \) can be approximated by the following equation.

\[ T_m = K_1 \left( h\nu_p \right)^{K_2} \]  

(6)

Where \( T_m \) in Kelvin and \( h\nu_p \) in eV, \( K_1 (\text{K/eV}) \) and \( K_2 \) (dimensionless) are constants for both II-VI and III-V semiconductors, such that 35.988 and 1.387, respectively.

On the other hand Kumar et al. [18] have proposed a parabolic equation for lattice energy in terms of plasmon energy, which is applicable for both II-VI and III-V semiconductors, and is given as
\[ U = a_i + b_i\left( \hbar w_p \right) - C_i \left( \hbar w_p \right)^2 \]  \hspace{1cm} (7)

Using equations (7) and (6) obtained by us, together with the equation (1), we obtained following equation for linear thermal expansion coefficient in terms of only plasmon energy for II-VI semiconductors.

\[ \frac{a_i}{10^{-6}} = 583.50 \left( \hbar w_p \right)^4 - 60.80 \left[ 1 - 0.034 \left( \hbar w_p \right) \right] \]  \hspace{1cm} (8)

for III-V semiconductor

\[ \frac{a_i}{10^{-6}} = 583.50 \left( \hbar w_p \right)^{-1.4} - 149.28 \left[ 1 - 0.042 \left( \hbar w_p \right) \right] \]  \hspace{1cm} (9)

RESULT AND DISCUSSION:

The calculated values of melting temperature by using equation (6) for all the binary semiconductors under study, reported in table 1, together with the experimental values [19,20]. Our calculated values are in close agreement within 8% with the experimental values, except BeO, GaN, GaSb, InN and InSb.

The calculated values of linear thermal expansion coefficient of II-VI and III-V semiconductors by using equations (8) and (9) are reported in table 1. The calculated values of \( \alpha_L \), together with the Kumar et al. values and experimental values are reported in table 1. Our calculated values are in close agreement with the experimental as well as Kumar et al. Values although equation (8) and (9) far deviate from experimental values in some cases, but these equations are useful in the sense that we can predict the values of \( \alpha_L \) by knowing only the plasmon energy of binary semiconductors.

CONCLUSION:

The linear thermal expansion coefficient of binary semiconductors has been studied by Neumann [14], Kumar et al [15] and recently by Omar [16]. In all these approaches experimental values of melting temperature is required in the calculations of thermal expansion coefficients. Therefore we have related melting temperature with the plasmon energy by a power law. The results obtained are found in close agreement within eight percent with the experimental values. Using this relationship together with the theories [14]. We have obtained expressions for linear thermal expansion coefficient for binary semiconductors mentioned in equations (8 and 9), which do not require any experimental data except the Plasmon energy. Our proposed
To Study the dependency of linear thermal expansion coefficient and Melting... 455

relations are simple and useful as we can directly calculate these parameters by having knowledge of Plasmon energy for these semiconductors. The knowledge of these calculated parameters may play a very important role in the development of semiconductors devices such as lasers, modulators and light emitting diodes.

Table 1. The values of melting temperature $T_m$ (K) and linear thermal expansion coefficient $\alpha_L$ ($10^{-6}$ K$^{-1}$) at $T = 300$ K for binary semiconductors

<table>
<thead>
<tr>
<th>S. No.</th>
<th>Compound</th>
<th>$T_m$</th>
<th>$\alpha_L$</th>
<th>$\hbar\omega_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BeO</td>
<td>2800</td>
<td>3715</td>
<td>7.43</td>
</tr>
<tr>
<td>2</td>
<td>BeS</td>
<td>2293</td>
<td>2223</td>
<td>7.88</td>
</tr>
<tr>
<td>3</td>
<td>BeSe</td>
<td>1964</td>
<td>2047</td>
<td>8.72</td>
</tr>
<tr>
<td>4</td>
<td>BeTe</td>
<td>1570</td>
<td>1705</td>
<td>9.50</td>
</tr>
<tr>
<td>5</td>
<td>MgTe</td>
<td>1300</td>
<td>1259</td>
<td>7.31</td>
</tr>
<tr>
<td>6</td>
<td>ZnO</td>
<td>2250</td>
<td>2539</td>
<td>8.62</td>
</tr>
<tr>
<td>7</td>
<td>ZnS</td>
<td>2100</td>
<td>1792</td>
<td>7.08</td>
</tr>
<tr>
<td>8</td>
<td>ZnSe</td>
<td>1788</td>
<td>1655</td>
<td>7.92</td>
</tr>
<tr>
<td>9</td>
<td>ZnTe</td>
<td>1568</td>
<td>1508</td>
<td>8.22</td>
</tr>
<tr>
<td>10</td>
<td>CdS</td>
<td>1748</td>
<td>1526</td>
<td>7.03</td>
</tr>
<tr>
<td>11</td>
<td>CdSe</td>
<td>1512</td>
<td>1403</td>
<td>7.43</td>
</tr>
<tr>
<td>12</td>
<td>CdTe</td>
<td>1365</td>
<td>1277</td>
<td>5.85</td>
</tr>
<tr>
<td>13</td>
<td>BN</td>
<td>3000</td>
<td>3053</td>
<td>6.99</td>
</tr>
<tr>
<td>14</td>
<td>BP</td>
<td>2800</td>
<td>2577</td>
<td>6.83</td>
</tr>
<tr>
<td>15</td>
<td>BAs</td>
<td>2300</td>
<td>2319</td>
<td>7.82</td>
</tr>
<tr>
<td>16</td>
<td>AlN</td>
<td>2500</td>
<td>2787</td>
<td>7.82</td>
</tr>
<tr>
<td>17</td>
<td>AlP</td>
<td>2100</td>
<td>1783</td>
<td>5.16</td>
</tr>
<tr>
<td>18</td>
<td>AlAs</td>
<td>2013</td>
<td>1651</td>
<td>3.75</td>
</tr>
<tr>
<td>19</td>
<td>AlSb</td>
<td>1300</td>
<td>1363</td>
<td>2.55</td>
</tr>
<tr>
<td>20</td>
<td>GaN</td>
<td>1500</td>
<td>2621</td>
<td>13.41</td>
</tr>
<tr>
<td>21</td>
<td>GaP</td>
<td>1750</td>
<td>1761</td>
<td>6.89</td>
</tr>
<tr>
<td>22</td>
<td>GaAs</td>
<td>1510</td>
<td>1593</td>
<td>6.92</td>
</tr>
<tr>
<td>23</td>
<td>GaSb</td>
<td>980</td>
<td>1316</td>
<td>8.86</td>
</tr>
<tr>
<td>24</td>
<td>InN</td>
<td>1200</td>
<td>2113</td>
<td>–</td>
</tr>
<tr>
<td>25</td>
<td>InP</td>
<td>1330</td>
<td>1508</td>
<td>6.32</td>
</tr>
<tr>
<td>26</td>
<td>InAs</td>
<td>1215</td>
<td>1412</td>
<td>5.23</td>
</tr>
<tr>
<td>27</td>
<td>InSb</td>
<td>798</td>
<td>1229</td>
<td>7.01</td>
</tr>
</tbody>
</table>
REFERENCES:

[8] F. Chiker, B. Abbar, A. Tadjer, S. Bresson, B. Khelifa, C. Mathieu, Physica B
To Study the dependency of linear thermal expansion coefficient and Melting...


