Debye Characteristic Temperatures of Some Cubic Semiconductors

By J. K. D. Verma, B. D. Nag, and P. S. Nair

Saha Institute of Nuclear Physics, Calcutta, India


The Debye characteristic temperatures for some of the cubic semiconductors have been calculated using the VRHG approximation and the series expansion method as developed by Betts, Bhatia and Wyman. It has been found that the VRHG approximation is simpler than the series expansion method. The values obtained using this approximation are also, in general, in good agreement with the experimental values and the values obtained by some other workers.

The Debye characteristic temperature, \( \Theta_D \), is an important parameter in the study of a large number of solid state problems involving lattice vibrations, such as electrical resistivity, thermal conductivity and scattering of thermal neutrons. Because of its importance and the scarcity of available low temperature specific heat data, several methods have been developed to calculate it from a knowledge of elastic properties of solids. The Debye temperature from the theory of specific heats, is given by

\[
\Theta_D = \frac{h}{k} \left[ \frac{3 q N \Omega^{\frac{1}{3}}}{4 \pi \lambda M} \right]^{\frac{1}{3}} v_m
\]

where \( h \) is Planck’s constant, \( k \) is Boltzmann’s constant, \( N \) is Avogadro’s number, \( \lambda \) is density, \( M \) is the molecular weight of the solid, \( q \) is the number of atoms in the molecule and \( v_m \) is given by

\[
v_m = \left[ \frac{1}{3} \int \frac{d^3 \Omega}{3} \right] \left( \frac{1}{v_j} \right)^{\frac{1}{4}}
\]

where \( d\Omega \) is an element of solid angle and \( v_j \) denotes the velocities of propagation of low-frequency vibrations and as such are functions of direction. The subscript \( j \) numbers the solutions to the Christoffel’s equations for plane wave motion. Hence, the calculation of the Debye characteristic temperature by the above two equations is limited only by the difficulties in computing \( v_m \).

The solution of the integral in equation (2) by numerical methods although rigorous and exact, is by no means practicable unless one has access to a high speed computer. Tables such as have been published by DeLaunay \(^2\) may be used with advantage in case of certain crystals but their scope is limited as these tables besides involving tedious calculations, are applicable only to some of the high symmetry solids. The series expansion method of Hopf and Lechner \(^3\) as modified by Quimby and Sutton \(^4\) and Sutton \(^5\) although a useful procedure, is equally lengthy and tedious and is applicable only to cubic crystals. While this is immaterial in single cases, the time spent in calculation can become disproportionately large where a series of compounds has to be considered.

Houston’s \(^6\) method of series expansion as developed by Betts et al. \(^7\) a, \(^b\), relating \( \Theta_D \) to the elastic constants of the crystal, is no doubt more general but still lengthy calculations are to be done, depending upon the number of terms selected in the series expansion. Joshi and Mitra \(^8\) have calculated by this method the Debye temperatures of a large number of solids. The method of Betts et al. \(^7\) a will be discussed in some detail in the next section as it has been used in this paper for the calculation of Debye temperatures of cubic semiconductors.

In the case of isotropic crystals, the evaluation of \( v_m \) is very much simpler as equation (2) reduces to the simple form

\[
v_m = \left[ \frac{1}{5} \left( \frac{1}{v_x} + \frac{1}{v_y} + \frac{1}{v_z} \right) \right]^{\frac{1}{3}}
\]

where \( v_x \) and \( v_y \) are the shear and longitudinal sound velocities and are related to the elastic constants of the solid.

4 S. L. Quimby and P. M. Sutton, Phys. Rev. 91, 1122 [1953].
5 P. M. Sutton, Phys. Rev. 99, 1826 [1955].
6 W. V. Houston, Rev. Mod. Phys. 20, 161 [1948].
Reddy has calculated the Debye temperatures for some of the substances, using calculated or experimental values of the velocities of propagation of longitudinal and torsional waves. The average error between the experimental and calculated values of $\Theta_D$ was up to 15 percent, barring the very large errors in case of substances like magnesium, molybdenum, cobalt, and silver chloride.

A number of approximate methods have also been developed. Born and Karman obtained a simplified expression to equation (2) when the crystals are nearly isotropic, viz.,

$$\frac{3}{v_m^3} = \rho^{\frac{3}{4}} [2(C_{44})^{-\frac{1}{4}} + (C_{22})^{-\frac{1}{4}}]$$

$$+ \left(\frac{3}{5}\right)(C_{12} - C_{11} + 2C_{44}) (C_{44}^{\frac{1}{4}} - C_{11}^{\frac{1}{4}})$$

where $C_{ij}$'s represent single crystal moduli.

Blackman suggested the following approximate method when the ratios $C_{12}/C_{11}$ and $C_{44}/C_{11}$ are small which seems to give good results.

$$v_m = \left[ C_{11} C_{44}^2 / \rho^3 \right]^{\frac{1}{4}}.$$  

Another approximate formula by Blackman covers those cases where the ratio $(C_{11} - C_{12})/C_{11}$ is very small and $\Theta_D$ is given by the relation

$$\Theta_D^3 = \frac{3 \cdot 15}{8 \pi} \left( \frac{h^3}{k} \right) \rho^{\frac{3}{4}} A$$

$$\cdot (C_{11} - C_{12})^{\frac{1}{4}} (C_{11} + C_{12} + 2C_{44})^{\frac{1}{4}} (C_{44})^{\frac{1}{2}}$$

where $A$ is the cell volume and $S$ is the number of atoms per unit cell.

These approximations are sometimes accurate but cannot be applied generally. Post has developed an approximation to avoid the complexities of anisotropy but it yields results which are considerably erroneous. Marcus and Kennedy investigated the relation between the elastic constants and the Debye temperatures at 0 K in the Debye approximation. They derived for cubic crystals the following expression,

$$\Theta_D(0) = 2.515 \times 10^{-3} C_{44} M^{-\frac{1}{2}} \rho^{-\frac{1}{4}} f(r_1, r_2)$$

where $M$ is the average “molecular weight” of the atoms in the crystal and

$$f(r_1, r_2) = \left[ \frac{1}{12 \pi} \int_{4\pi} \sum_{j=1}^{3} v_j^2 d\Omega \right]^{-\frac{1}{3}},$$

$$r_1 = (C_{11} - C_{12})/2C_{11} ; \quad r_2 = C_{44}/C_{11} ; \quad v_j = v_j/v_0,$$

$$v_0 = (C_{11}/\rho)^{\frac{1}{3}}.$$  

Their calculation of the Debye temperature of Ge, though lengthy shows perfect agreement with the result of low-temperature specific heat data. Anderson has calculated the Debye temperatures of a large number of crystals of different structures, using VRHG approximation. The accuracy obtained by this method is quite good besides being simpler. The method will be described in more detail later in section 2 as it has also been utilized in this paper for the calculation of Debye temperatures.

There have also been several attempts to estimate the unknown Debye temperatures using simple parameters such as the atomic or molecular weight, lattice constant, melting point (cf. Blackman). Recently, Steigmeier has modified equation (7) for estimating the Debye temperatures of zincblende lattice type semiconductors using the observation of Keys that the elastic constants of some group IV, III – V and II – VI elements and compounds are functions of their lattice parameters only. The final expression can be written as

$$\Theta_D(0) = [4.19 \times 10^{-8}/(a_0^3M)] G$$

where $a_0$ is the lattice parameter and the quantity

$$G = \left[ \frac{3}{16 \pi} \left( C_{11} \right)^{\frac{1}{2}} f(r_1, r_2) \right]$$

varies very little with $a_0$. Using the experimental values of only four of the III – V semiconductor compounds, Steigmeier has been able to predict the $\Theta_D(0)$ values of the remaining zincblende structure III – V compounds. There are several other approximations available in the literature but they either lack generality or accuracy.

So far the Debye temperatures reported in the literature are mostly for metals and other compounds, similar data for semiconductors being very scarce. The object of this paper is to calculate the Debye temperature of Ge using approximate methods available in the literature.

References:

8b J. K. D. Verma, B. D. N. Nag, and P. S. Nair, Physica 29, 63 [1963].
9 M. Born and T. T. Karman, Phys. Z., 14, 15 [1913].
11 M. Blackman, Phil. Mag. 42, 1441 [1951].
17b Except for III–V compounds for which U. Piesbergen (Z. Naturforsch. 18a, 141 [1963]) has calculated from the experimentally measured values of atomic heats between 10 and 273 K.
Debye temperatures of some semiconductors having cubic structure, using VRHG approximation and the method of Betts et al.\textsuperscript{7} as these methods are quite general and applicable to crystals of all classes. The Debye temperatures of non cubic semiconductors will be presented in a later publication.

1. Method of Betts, Bhatia and Wyman for the Calculation of Debye Temperatures

Houston\textsuperscript{6} gave a convenient method for approximately determining the frequency distribution of cubic crystals. Later, Betts et al.\textsuperscript{7a,b} modified it for application to include non cubic crystals. The expression for the Debye temperature for cubic crystals in terms of the elastic constants is given by

\[ \Theta_D = \frac{h}{k} \left( \frac{9S}{\lambda} \right) J_m^{-\lambda} \]  

(9)

where the symbols have their usual meaning and \( J_m \) is given by any of the following expressions, depending upon the number of terms taken in the expansion.

\[
\begin{align*}
J_1 &= \frac{4\pi}{35} \left[ 10A + 16B + 9C \right], \\
J_2 &= \frac{4\pi}{945} \left[ 45A + 32B + 243C + 625D \right], \\
J_3 &= \frac{4\pi}{35} \left[ 6A + 8B - 3C + 24E \right], \\
J_4 &= \frac{4\pi}{70} \left[ 17A - 64B - 126C + 243F \right], \\
J_5 &= \frac{4\pi}{10395} \left[ 1197A + 1456B + 729C + 3125D + 3888E \right], \\
J_6 &= \frac{4\pi}{83160} \left[ 7281A - 13312B - 13608C + 59049F + 43750D \right], \\
J_7 &= \frac{4\pi}{770} \left[ 117A + 416B + 294C + 672E - 729F \right], \\
J_8 &= \frac{4\pi}{1081080} \left[ 117603A + 76544B + 17496C + 381250D + 311040E + 177147F \right],
\end{align*}
\]

(10)

where

\[
\begin{align*}
A &= \phi^{-\lambda} \left[ 2(C_{44})^{-\lambda} + (C_{44} + \alpha)^{-\lambda} \right], \\
B &= \phi^{-\lambda} \left[ (C_{44})^{-\lambda} + \{C_{44} + \frac{1}{3}(\alpha - \beta)\}^{-\lambda} + \{C_{44} + \frac{1}{3}(\alpha + \beta)\}^{-\lambda} \right], \\
C &= \phi^{-\lambda} \left[ 2 \{C_{44} + \frac{1}{3}(\alpha - \beta)\}^{-\lambda} + \{C_{44} + \frac{1}{3}(\alpha + 2\beta)\}^{-\lambda} \right], \\
D &= \phi^{-\lambda} \left[ (C_{44})^{-\lambda} + \{C_{44} + \frac{1}{3} \alpha + \frac{1}{10} (9 \alpha^2 + 16 \beta^2) \}^{-\lambda} + \{C_{44} + \frac{1}{3} \alpha - \frac{1}{10} (9 \alpha^2 + 16 \beta^2) \}^{-\lambda} \right], \\
E &= \phi^{-\lambda} \left[ \{C_{44} + \frac{1}{3} (\alpha - \beta)\}^{-\lambda} + \{C_{44} + \frac{1}{3} (5 \alpha + \beta) + \frac{1}{10} (9 \alpha^2 + 33 \beta^2 - 6 \alpha \beta) \}^{-\lambda} \\
&\quad + \{C_{44} + \frac{1}{3} (5 \alpha + \beta) - \frac{1}{10} (9 \alpha^2 + 33 \beta^2 - 6 \alpha \beta) \}^{-\lambda} \right], \\
F &= \phi^{-\lambda} \left[ \{C_{44} + \frac{1}{3} (\alpha - \beta)\}^{-\lambda} + \{C_{44} + \left( \frac{1}{10} (9 \alpha^2 + 48 \beta^2 + 24 \alpha \beta) \right) \}^{-\lambda} \\
&\quad + \{C_{44} + \left( \frac{1}{10} (9 \alpha^2 + 48 \beta^2 + 24 \alpha \beta) \right) \}^{-\lambda} \right], \\
\alpha &= C_{11} - C_{44}, \quad \beta = C_{12} + C_{44}.
\end{align*}
\]

The expression \( J_1 \) is known as Houston's approximation. The Debye temperatures have been calculated using equations (9) and (10) and have been designated \( \Theta_1, \Theta_2, \Theta_3, \ldots, \Theta_8 \) corresponding to \( J_1, J_2, J_3, \ldots J_8 \). It has been shown by Betts et al.\textsuperscript{7a} that in case \( \eta = 2C_{44}/(C_{11} - C_{12}) \) lies between 0.5 and 1.5, Houston's approximation is not in error by more than a fraction of a percent.
2. VRHG Approximation for Calculating Debye Temperatures

This method of averaging the elastic constants and sound velocities is a synthesis of various relations and ideas given by Voigt\(^{18}\), Reuss\(^{19}\), Hill\(^{20}\) and Gilvarry\(^{21}\) (VRHG). Voigt\(^{18}\) showed that a simple linear relation exists between isotropic shear (K) and bulk (G) moduli and single crystal moduli \((C_{ij})^*\), viz.

\[
K_V = \frac{1}{3} (C_{11} + C_{22} + C_{33}) + \frac{2}{3} (C_{12} + C_{23} + C_{13}),
\]

\[
G_V = \frac{1}{3} (C_{11} + C_{22} + C_{33}) - \frac{1}{9} (C_{12} + C_{23} + C_{13})
+ \frac{1}{3} (C_{44} + C_{55} + C_{66}).
\]  

Reuss\(^{19}\) obtained, however, a different set of relations for K and G which are

\[
(K_R)^{-1} = (S_{11} + S_{22} + S_{33}) + 2(S_{12} + S_{23} + S_{13}),
\]

\[
15(G_R)^{-1} = 4(S_{11} + S_{22} + S_{33}) - 4(S_{12} + S_{23} + S_{13})
+ 3(S_{44} + S_{55} + S_{66}).
\]

where \(S_{ij}\)'s represent compliance.

In case of cubic crystals, \(C_{ij}\) and \(S_{ij}\) are related by the following expressions (cf. Kittel\(^{22}\))

\[
C_{11} = (S_{11} + S_{12})/(S_{11} - S_{12}),
\]

\[
C_{12} = -S_{12}/(S_{11} - S_{12}),
\]

\[
C_{44} = 1/S_{44},
\]

\[
S_{11} = (C_{11} + C_{12})/(C_{11} - C_{12}),
\]

\[
S_{12} = -C_{12}/(C_{11} - C_{12}),
\]

\[
S_{44} = 1/C_{44}.
\]  

Hill\(^{20}\) has shown that the values of K and G obtained by Voigt and Reuss represent the maximum and minimum limits of these quantities respectively and suggested for a good estimate of these moduli to take the arithmetic mean of these extremes. Thus,

\[
K_H = \frac{1}{2} (K_V + K_R),
\]

\[
G_H = \frac{1}{2} (G_V + G_R).
\]  

The average sound velocities, \(\bar{v}_s\) and \(\bar{v}_l\) can then be computed from the following relations:

\[
\bar{v}_s = (G_H/q)^{1/3},
\]

\[
\bar{v}_l = [(K_H + \frac{4}{3} G_H)/q]^{1/2}.
\]

Substituting these values of \(\bar{v}_s\) and \(\bar{v}_l\) in equation (3), one obtains an average value \(\bar{v}_m\) which is little different from \(v_m\) calculated by the rigorous method.

\[
\bar{v}_m = \left[(2\bar{v}_s^{-3} + \bar{v}_l^{-3})/3\right]^{-1/3}.
\]  

Gilvarry\(^{21}\) was the first to calculate by this method the Debye temperature of sodium. It was, however, Anderson\(^{14}\), who computed the exact value of \(v_m\) with the help of a IBM 7090 computer and arrived at the conclusion that it makes no substantial difference in the ultimate value of \(\Theta_D\) by accepting the average value, \(\bar{v}_m\) instead of the more rigorous and exact value \(v_m\). He also showed experimentally that the average values of K and G obtained by equation (14) are close in values to those obtained on polycrystalline hot pressed sintered materials. He pointed out that for degree of anisotropy, \(\delta\), less than 20 percent, the approximation error, \(\xi\), is less than 2 percent where these quantities are defined as

\[
\delta = \frac{3(2C_{44} - (C_{11} - C_{12}))^2}{12C_{44}^2 + 38C_{44}(C_{11} - C_{12}) + 3(C_{11} - C_{12})^2},
\]

\[
\xi = (\bar{v}_m - v_m)/v_m.
\]  

The relationship between \(\xi\) and \(\delta\) permits a rather exact estimate of the Debye temperature from the elastic constants of a cubic crystal. Using equations (1) and (11) to (16), Anderson\(^{14}\) has calculated the Debye temperatures of more than 200 crystals of all classes.

3. Results

The Debye characteristic temperatures have been calculated for some of the cubic semiconductors, using VRHG approximation and the series expansion method of Betts, Bhatia and Wyman\(^{7,a}\). Although there are more than sixty semiconductors having cubic structure (cf. Lawson and Nielsen\(^{23}\)), the Debye temperatures have been reported here for only seventeen of them. This is due to the non availability of elastic and lattice constants data.

Sometimes widely differing values for these data have been used for the same material by various authors in the calculation of Debye temperatures and hence, it has been somewhat difficult to com-

* For cubic crystals, \(C_{11} = C_{22} = C_{33}\), \(C_{44} = C_{55} = C_{66}\), and \(C_{12} = C_{23} = C_{13}\).


\(^{19}\) A. Reuss, Z. angew. Math. Mech. 9, 55 [1929].


\(^{21}\) J. J. Gilvarry, 1956, Phys. Rev. 103, 1700 [1956].


## Debye Temperatures of Some Semiconductors

### Table 1. Parameters Used in the Calculation of Debye Temperatures of Cubic Semiconductors.

<table>
<thead>
<tr>
<th>Material</th>
<th>Elastic Constants</th>
<th>Lattice Constant</th>
<th>Density</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$C_{11}$</td>
<td>$C_{12}$</td>
<td>$C_{44}$</td>
</tr>
<tr>
<td>C</td>
<td>94.90</td>
<td>10.50</td>
<td>52.10</td>
</tr>
<tr>
<td>Si</td>
<td>16.56</td>
<td>6.386</td>
<td>7.953</td>
</tr>
<tr>
<td>Ge</td>
<td>12.88</td>
<td>4.825</td>
<td>6.705</td>
</tr>
<tr>
<td>AlSb</td>
<td>8.94</td>
<td>4.43</td>
<td>4.15</td>
</tr>
<tr>
<td>GaAs</td>
<td>11.88</td>
<td>5.38</td>
<td>5.94</td>
</tr>
<tr>
<td>GaSb</td>
<td>8.85</td>
<td>4.04</td>
<td>4.32</td>
</tr>
<tr>
<td>InAs</td>
<td>8.329</td>
<td>4.526</td>
<td>3.959</td>
</tr>
<tr>
<td>InSb</td>
<td>6.717</td>
<td>3.665</td>
<td>3.018</td>
</tr>
<tr>
<td>ZnS</td>
<td>10.79</td>
<td>7.22</td>
<td>4.12</td>
</tr>
<tr>
<td>ZnSe</td>
<td>8.10</td>
<td>4.88</td>
<td>4.41</td>
</tr>
<tr>
<td>ZnTe</td>
<td>7.13</td>
<td>4.07</td>
<td>3.12</td>
</tr>
<tr>
<td>CdTe</td>
<td>5.551</td>
<td>3.681</td>
<td>1.994</td>
</tr>
<tr>
<td>MgSi</td>
<td>10.46</td>
<td>1.67</td>
<td>4.25</td>
</tr>
<tr>
<td>MgGe</td>
<td>10.43</td>
<td>1.41</td>
<td>4.30</td>
</tr>
<tr>
<td>PbS</td>
<td>12.70</td>
<td>2.98</td>
<td>2.48</td>
</tr>
<tr>
<td>FeS$_2$</td>
<td>36.20</td>
<td>10.40</td>
<td>1.300</td>
</tr>
<tr>
<td>PbTe</td>
<td>10.72</td>
<td>0.768</td>
<td>1.300</td>
</tr>
</tbody>
</table>

### Table 2. Debye Temperature Using the Method of Betts, Bhatia, and Wyman.

<table>
<thead>
<tr>
<th>Material</th>
<th>Anisotropy Factor $\eta$</th>
<th>$\Theta_1$</th>
<th>$\Theta_2$</th>
<th>$\Theta_3$</th>
<th>$\Theta_4$</th>
<th>$\Theta_5$</th>
<th>$\Theta_6$</th>
<th>$\Theta_7$</th>
<th>$\Theta_8$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>1.303</td>
<td>1995.0</td>
<td>2290.7</td>
<td>1894.4</td>
<td>1603.8</td>
<td>2014.8</td>
<td>2026.1</td>
<td>2033.9</td>
<td>1986.1</td>
</tr>
<tr>
<td>Si</td>
<td>1.733</td>
<td>573.7</td>
<td>558.2</td>
<td>576.8</td>
<td>555.9</td>
<td>508.5</td>
<td>581.6</td>
<td>569.6</td>
<td>575.4</td>
</tr>
<tr>
<td>Ge</td>
<td>1.663</td>
<td>343.6</td>
<td>336.2</td>
<td>359.4</td>
<td>325.6</td>
<td>348.5</td>
<td>358.3</td>
<td>368.5</td>
<td>346.8</td>
</tr>
<tr>
<td>AlSb</td>
<td>1.840</td>
<td>270.3</td>
<td>273.2</td>
<td>271.7</td>
<td>286.1</td>
<td>272.7</td>
<td>299.8</td>
<td>254.0</td>
<td>276.7</td>
</tr>
<tr>
<td>GaAs</td>
<td>1.827</td>
<td>368.1</td>
<td>345.4</td>
<td>309.7</td>
<td>330.9</td>
<td>341.5</td>
<td>314.5</td>
<td>351.9</td>
<td>324.2</td>
</tr>
<tr>
<td>GaSb</td>
<td>1.842</td>
<td>265.7</td>
<td>233.1</td>
<td>179.4</td>
<td>246.4</td>
<td>231.8</td>
<td>258.5</td>
<td>244.8</td>
<td>235.6</td>
</tr>
<tr>
<td>InAs</td>
<td>2.132</td>
<td>239.4</td>
<td>238.9</td>
<td>211.5</td>
<td>233.4</td>
<td>236.1</td>
<td>243.6</td>
<td>239.5</td>
<td>235.6</td>
</tr>
<tr>
<td>InSb</td>
<td>1.974</td>
<td>181.0</td>
<td>186.2</td>
<td>178.8</td>
<td>185.1</td>
<td>180.9</td>
<td>185.8</td>
<td>174.4</td>
<td></td>
</tr>
<tr>
<td>ZnS</td>
<td>2.308</td>
<td>293.7</td>
<td>298.2</td>
<td>299.4</td>
<td>297.2</td>
<td>303.9</td>
<td>304.3</td>
<td>300.3</td>
<td>303.3</td>
</tr>
<tr>
<td>ZnSe</td>
<td>2.739</td>
<td>251.5</td>
<td>248.0</td>
<td>247.4</td>
<td>241.3</td>
<td>245.7</td>
<td>246.7</td>
<td>244.8</td>
<td>245.9</td>
</tr>
<tr>
<td>ZnTe</td>
<td>2.039</td>
<td>201.3</td>
<td>214.3</td>
<td>200.1</td>
<td>198.8</td>
<td>206.1</td>
<td>210.7</td>
<td>198.3</td>
<td>207.1</td>
</tr>
<tr>
<td>CdTe</td>
<td>2.338</td>
<td>140.6</td>
<td>143.2</td>
<td>143.0</td>
<td>193.2</td>
<td>143.8</td>
<td>148.8</td>
<td>143.2</td>
<td>145.1</td>
</tr>
<tr>
<td>MgSi</td>
<td>0.967</td>
<td>443.9</td>
<td>444.1</td>
<td>443.3</td>
<td>461.9</td>
<td>443.7</td>
<td>447.4</td>
<td>439.0</td>
<td>444.4</td>
</tr>
<tr>
<td>MgGe</td>
<td>0.933</td>
<td>352.8</td>
<td>362.1</td>
<td>352.8</td>
<td>358.7</td>
<td>327.1</td>
<td>335.8</td>
<td>351.2</td>
<td>353.0</td>
</tr>
<tr>
<td>PbS</td>
<td>0.510</td>
<td>206.4</td>
<td>197.5</td>
<td>209.5</td>
<td>234.3</td>
<td>216.0</td>
<td>212.1</td>
<td>205.3</td>
<td>210.5</td>
</tr>
<tr>
<td>FeS$_2$</td>
<td>0.512</td>
<td>556.9</td>
<td>561.4</td>
<td>562.5</td>
<td>569.7</td>
<td>566.0</td>
<td>563.2</td>
<td>561.1</td>
<td>562.4</td>
</tr>
<tr>
<td>PbTe</td>
<td>0.261</td>
<td>141.4</td>
<td>142.5</td>
<td>149.7</td>
<td>161.1</td>
<td>146.0</td>
<td>146.0</td>
<td>146.1</td>
<td>146.1</td>
</tr>
</tbody>
</table>

Where $M$ is the atomic (or molecular) weight of the substance and $S$ is the number of atoms (or molecules) per unit cell. In case of cubic crystals, $S=3$ for elemental and $S=4$ for compound semiconductors.
The parameters used in the calculation of Debye temperatures of cubic crystals are $C_{11}$, $C_{12}$, $C_{44}$, $a_0$, $q$ and these have been presented in Table 1.

The elastic constants data for all these semiconductors are at room temperature. The crystals have been divided into three groups – elemental (group IV), compounds from group III – V and compounds from other groups such as II – VI; IV – VI, etc.

The eight different values of the Debye temperatures, $\Theta_1$, ..., $\Theta_8$, for each crystal obtained by the method of Betts et al. have been presented in Table 2.

The values of the Debye temperatures obtained by VRHG approximation and Houston’s approximation viz. $\Theta_1$, have been tabulated for the sake of comparison in Table 3, along with the values taken from other sources. Only the value given by Houston’s approximation was selected for comparison since besides being simpler to compute than any of other seven values $\Theta_2$, ..., $\Theta_8$, the accuracy is also quite comparable.

### Table 2

<table>
<thead>
<tr>
<th>Material</th>
<th>HOUSTON’S Approximation</th>
<th>VRHG Approximation</th>
<th>STEIGMEIER’S Approximation</th>
<th>S. C. S.*</th>
<th>A. I. P.**</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>1995</td>
<td>2167</td>
<td>—</td>
<td>2240</td>
<td>2240</td>
</tr>
<tr>
<td>Si</td>
<td>573.7</td>
<td>637</td>
<td>—</td>
<td>639</td>
<td>645</td>
</tr>
<tr>
<td>Ge</td>
<td>343.6</td>
<td>377.5</td>
<td>—</td>
<td>400</td>
<td>374</td>
</tr>
<tr>
<td>AlSb</td>
<td>270.3</td>
<td>290.3</td>
<td>292</td>
<td>370</td>
<td>—</td>
</tr>
<tr>
<td>GaAs</td>
<td>312.5</td>
<td>348.6</td>
<td>344</td>
<td>355</td>
<td>—</td>
</tr>
<tr>
<td>GaSb</td>
<td>237.9</td>
<td>267.5</td>
<td>263.5</td>
<td>250</td>
<td>—</td>
</tr>
<tr>
<td>InAs</td>
<td>225.6</td>
<td>246.4</td>
<td>262</td>
<td>270</td>
<td>—</td>
</tr>
<tr>
<td>InSb</td>
<td>183.4</td>
<td>205.6</td>
<td>202.5</td>
<td>170</td>
<td>—</td>
</tr>
<tr>
<td>ZnS</td>
<td>293.7</td>
<td>331.3</td>
<td>—</td>
<td>315</td>
<td>—</td>
</tr>
<tr>
<td>ZnSe</td>
<td>251.5</td>
<td>232.8</td>
<td>—</td>
<td>400</td>
<td>—</td>
</tr>
<tr>
<td>ZnTe</td>
<td>201.3</td>
<td>217.4</td>
<td>—</td>
<td>250</td>
<td>—</td>
</tr>
<tr>
<td>CdTe</td>
<td>140.6</td>
<td>159.2</td>
<td>—</td>
<td>200</td>
<td>—</td>
</tr>
<tr>
<td>Mg²Si</td>
<td>443.9</td>
<td>551.2</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>MgGe</td>
<td>352.8</td>
<td>441.4</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>PbS</td>
<td>206.4</td>
<td>233.5</td>
<td>—</td>
<td>—</td>
<td>194</td>
</tr>
<tr>
<td>FeS₂</td>
<td>556.9</td>
<td>717.7</td>
<td>—</td>
<td>—</td>
<td>645</td>
</tr>
<tr>
<td>PbTe</td>
<td>141.4</td>
<td>171.3</td>
<td>—</td>
<td>137</td>
<td>—</td>
</tr>
</tbody>
</table>

### Table 3. Comparison of Debye Temperatures.

* Selected Constants Relative to Semiconductors.
** American Institute of Physics Handbook.

### 4. Discussion

The elastic constants presented in Table 1 were selected on the basis of reliability of data where different values were quoted. Except in the case of diamond in which case the values differed very much — $C_{11}$ varied from 95 to 110, $C_{12}$ from 12 to 33 and $C_{44}$ from 43 to 58 (cf. Huntington) – the values quoted generally differed in the first or second decimal places. This may correspond to an error of about 1 percent in $\Theta_D$ value. It has also been found that very few authors presented density data along with the elastic constants while reporting calculation of Debye $\Theta$ using a particular method. This is important since a slight difference in $q$ value — $C_{ij}$ values remaining same — will give rise to another 1 percent error in the value of the Debye temperature. This is evident from the result of Joshi and Mitra on the calculation of Debye $\Theta$ of GaAs using Houston’s approximation where they used the same elastic constants as in the present work but report a value of 314 °K while in the present work it comes out to be 312.49 °K. This may be due to the difference in the density values. Though the difference between the two $\Theta_D$ values is negligibly small, one should not forget that the $\Theta_D$ values calculated by some of the approximate methods differ by this amount. Hence the accuracy claimed by a particular method has to be viewed with caution.

The error introduced by using elastic constants at room temperature instead of the value at 0 °K is also about 1 percent due to the small variation of the elastic constants in this temperature range.

The eight different values of $\Theta_D$, calculated by the method of Betts, Bhatia and Wyman and given in Table 2, do not, however, show any general systematics except for one or two features. It is seen that $\Theta_4$ value is always very much different from all other seven values. Also, for anisotropy factor $\eta > 2$, $\Theta_5$, $\Theta_6$, $\Theta_7$ and $\Theta_8$ are much closer to each other than $\Theta_1$, $\Theta_2$ and $\Theta_3$. The three term approximation viz., Houston’s approximation is, however, sufficient for a good estimate of the Debye temperature, besides being simpler and less time consuming.

The agreement between the $\Theta_D$ values obtained by VRHG approximation and the experimental values taken from the American Institute of Physics Handbook is quite good except in the case of diamond. In case of III – V compounds the values calculated using VRHG approximation also shows better agreement with the values reported by Steigmeier, than Houston’s approximation. The agreement is also quite good with the values obtained by Piesbergen. The values obtained by VRHG

approximation are always higher as compared with those by Houston’s approximation.

5. Conclusion

It has been found that VRHG approximation for the calculation of the Debye temperatures of cubic crystals is quite simple and gives accurate results in comparison with any of the other approximate methods. It takes about ten minutes on the slide rule to compute $\Theta_D$. The method is also general in that it is applicable to a crystal of any symmetry. Moreover, in this method the elastic parameters need not be that of a single crystal; such data on hot pressed sintered material will suffice for determining Debye $\Theta$.

Spinwellen in dünnen ferromagnetischen Schichten

Von Rainer J. Jelitto *

Institut für Theoretische Physik der Universität München
(Z. Naturforschg. 19 a, 1567—1580 [1964]; eingegangen am 31. Juli 1964)

This paper is concerned with an ideal spin-1/2-Heisenberg-model for thin ferromagnetic films. A general method is given for the calculation of the one-spinwave eigenstates and their spectrum in dependence on the lattice type and the orientation of the surfaces of the film. The function that characterises the shape of the spinwave perpendicular to the film must fulfil a linear eigenvalue-difference-equation as well as a set of boundary conditions.

For next-neighbour interactions this system may be evaluated for an especially simple case. For it spinwavestates of the form of cos-sin-functions as well as surface states are found. Their momenta are given by some transcendental equations, which are discussed.

For all other cases the given difference-equation cannot be solved in a closed form, but at any rate it is a starting point for numerical calculations.

In a subsequent paper it will be shown that the special case mentioned above covers some important surface orientations of the cubic lattice types. For films of these orientations the dependence of the magnetization on temperature and thickness of the film will be derived from the spinwave spectra.


Besonders bei niedrigen Temperaturen, bei denen das Konzept der Spinwellen ein angemessenes Bild liefert, führen bereits die einfachsten Näherungen zu guten Ergebnissen. Das so gewonnene Blochsche $T^{\mu\nu}$-Gesetz für die Temperaturabhängigkeit der spontanen Magnetisierung eines unendlich ausgedehnten dreidimensionalen Kristalls trägt dem tatsächlichen Verhalten dieser Größe gut Rechnung und wurde verschiedentlich experimentell bestätigt. Bei Rechnungen über das Flächengitter und die lineare Kette kommt es zu Divergenzen, deren tiefliegende Ursachen im Falle des Flächengitters erst 1961 durch Döring geklärt werden konnten.

Legt man den Untersuchungen ein allseitig unendlich ausgedehntes Kristallgitter zugrunde, so werden die Rechnungen durch die Translationsinvariante des Hamilton-Operators erheblich vereinfacht; allerdings beginnt man sich damit in bekannter Weise der Erfassung von Oberflächeneffekten. Doch ist die Anwendbarkeit des Heisenberg-Modells und Spinwellenkonzeptes keineswegs auf translationsinvariante Probleme beschränkt; wenn man die besonderen Verhältnisse berücksichtigt, welche die Spins in der Nähe von Oberflächen dadurch antreffen, daß sie weniger Nachbarn besitzen als innere Gitterpunkte, sind sie auch zur Beschreibung von Oberflächeneffekten geeignet.

* Jetzt Institut für Theoretische Physik der Universität Kiel.


2 F. Bloch, Z. Phys. 61, 206 [1930].

3 S. Foxer u. E. D. Thompson, J. Appl. Phys. 30, 229 [1959].


5 W. Döring, Z. Naturforschg. 16 a, 1008 [1961].