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, Θ_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 the relation [1]

$$\Theta_D = \frac{h}{k} \left[\frac{3\,q}{4\,\pi} \frac{N\,\varrho}{M} \right]^{1/3} v_m \qquad (1)$$

where h is Planck's constant, k is Boltzmann's constant, N is Avogadro's number, ϱ 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

$$v_m = \left[\frac{1}{3} \int \sum_{j=1}^{3} \frac{1}{v_j{}^3} \frac{d\Omega}{4\,\pi} \right]^{-1/3} \qquad (2)$$

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 Θ_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 [8a] 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

$$v_m = \left[(2\,v_s{}^{-3} + v_l{}^{-3})/3 \right]^{-1/3} \qquad (3)$$

where v_s and v_l are the shear and longitudinal sound velocities and are related to the elastic constants of the solid.

[1] H. B. Huntington, Solid State Physics (edited by F. Seitz and D. Turnbull), 7, Academic Press, New York 1958.
[2] J. DeLaunay, Solid State Physics (edited by F. Seitz and D. Turnbull), 2, Academic Press, New York 1958.
[3] L. Hopf and G. Lechner, Verh. dtsch. Phys. Ges. 16, 643 [1914].
[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].
[7] a) D. D. Betts, A. B. Bhatia, and M. Wyman, Phys. Rev. 104, 37 [1956]. — b) D. D. Betts, A. B. Bhatia, and G. K. Horton, Phys. Rev., 104, 43 [1956].
[8a] S. K. Joshi and S. S. Mitra, Proc. Phys. Soc., Lond. 76, 295 [1960].

REDDY [8b] 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 Θ_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 [9] obtained a simplified expression to equation (2) when the crystals are nearly isotropic, viz.,

$$\frac{3}{v_\mathrm{m}^3} = \varrho^{3/2} [2\,(C_{44})^{-3/2} + (C_{22})^{-3/2}$$

$$+ (\tfrac{3}{5})\,(C_{12} - C_{11} + 2\,C_{44})\,(C_{44}^{-5/2} - C_{11}^{-5/2})]\tag{4}$$

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

BLACKMAN [10 a, b] 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.

$$v_\mathrm{m} = [C_{11}\,C_{44}^2/\varrho^3]^{1/6}.\tag{5}$$

Another approximate formula by BLACKMAN [11] covers those cases where the ratio $(C_{11} - C_{12})/C_{11}$ is very small and Θ_D is given by the relation

$$\Theta_\mathrm{D}^3 = \frac{3\cdot 15}{8\,\pi} \left(\frac{h}{k}\right)^3 \frac{S}{\varrho^{3/2}\,\Delta}$$

$$\cdot (C_{11} - C_{12})^{1/2} (C_{11} + C_{12} + 2\,C_{44})^{1/2} (C_{44})^{1/2}\tag{6}$$

where Δ 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 [12] has developed an approximation to avoid the complexities of anisotropy but it yields results which are considerably erraneous. MARCUS and KENNEDY [13] investigated the relation between the elastic constants and the DEBYE temperatures at $0\,°\mathrm{K}$ in the DEBYE approximation. They derived for cubic crystals the following expression,

$$\Theta_\mathrm{D}(0) = 2.515 \times 10^{-3}\,C_{11}^{1/2}\,M^{-1/3}\,\varrho^{-1/6}\,f(r_1, r_2)\tag{7}$$

where M is the average "molecular weight" of the atoms in the crystal and

$$f(r_1, r_2) = \left[\frac{1}{12\,\pi} \int\limits_{4\pi} \sum_{j=1}^3 v_{rj}^{-3}\,\mathrm{d}\Omega\right]^{-1/3},$$

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

$$v_{rj} = v_j/v_0, \qquad v_0 = (C_{11}/\varrho)^{1/2}.$$

Their calculation of the DEBYE temperature of Ge, though lengthy shows perfect agreement with the result of low-temperature specific heat data. ANDERSON [14] 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 [15]). Recently, STEIGMEIER [16] has modified equation (7) for estimating the DEBYE temperatures of zincblende lattice type semiconductors using the observation of KEYES [17a] 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

$$\Theta_\mathrm{D}(0) = [4.19 \times 10^{-8}/(a_0^3\,M)^{1/2}] \cdot G\tag{8}$$

where a_0 is the lattice parameter and the quantity

$$G = \left[\frac{3\,a_0^2}{16\,e}\,(C_{11})^{1/2}\,f(r_1, r_2)\right]$$

varies very little with a_0. Using the experimental values of only four of the III − V semiconductor compounds, STEIGMEIER [16] has been able to predict the $\Theta_\mathrm{D}(0)$ 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 scarse [17b]. The object of this paper is to calculate the

[8b] P. J. REDDY, Physica **29**, 63 [1963].
[9] M. BORN and T. T. KARMAN, Phys. Z., **14**, 15 [1913].
[10] a) M. BLACKMAN, Proc. Roy. Soc., Lond. A **148**, 384 [1935]. − b) M. BLACKMAN, ibid. A **149**, 126 [1935].
[11] M. BLACKMAN, Phil. Mag. **42**, 1441 [1951].
[12] E. J. POST, Canad. J. Phys. **21**, 112 [1953].
[13] P. M. MARCUS and A. J. KENNEDY, Phys. Rev. **114**, 459 [1959].
[14] O. L. ANDERSON, J. Phys. Chem. Solids **24**, 909 [1963].

[15] M. BLACKMAN, Handbuch der Physik (edited by S. FLÜGGE), **VII**, Part I, Springer-Verlag, Berlin 1955.
[16] E. F. STEIGMEIER, Appl. Phys. Letters **3**, 6 [1963].
[17a] R. W. KEYES, J. Appl. Phys. **33**, 3371 [1962].
[17b] Except for III − V compounds for which U. PIESBERGEN (Z. Naturforsch. **18 a**, 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.[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[6] gave a convenient method for approximately determining the frequency distribution of cubic crystals. Later, BETTS et al.[7 a, 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

$$\Theta_\mathrm{D} = \frac{h}{k}\left(\frac{9S}{\Delta}\right)^{1/3} J_\mathrm{m}^{-1/3} \qquad (9)$$

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

$$
\begin{aligned}
J_1 &= \frac{4\pi}{35}\left[\ \ 10\,A + \ \ 16\,B + \ \ \ 9\,C\right], \\[4pt]
J_2 &= \frac{4\pi}{945}\left[\ \ 45\,A + \ \ 32\,B + \ \ 243\,C + 625\,D\right], \\[4pt]
J_3 &= \frac{4\pi}{35}\left[\ \ \ 6\,A + \ \ \ 8\,B - \ \ \ 3\,C + \ 24\,E\right], \\[4pt]
J_4 &= \frac{4\pi}{70}\left[\ \ 17\,A - \ \ 64\,B - \ 126\,C + 243\,F\right], \\[4pt]
J_5 &= \frac{4\pi}{10395}\left[\ 1197\,A + \ 1456\,B + \ \ 729\,C + \ \ 3125\,D + 3888\,E\right], \\[4pt]
J_6 &= \frac{4\pi}{83160}\left[\ 7281\,A - 13312\,B - 13608\,C + 59049\,F + 43750\,D\right], \\[4pt]
J_7 &= \frac{4\pi}{770}\left[\ 117\,A + \ 416\,B + \ 294\,C + \ 672\,E - \ 729\,F\right], \\[4pt]
J_8 &= \frac{4\pi}{1081080}\left[117603\,A + 76\,544\,B + 17496\,C + 381250\,D + 311040\,E + 177147\,F\right]
\end{aligned}
$$

$$(10)$$

where

$$A = \varrho^{3/2}[2\,(C_{44})^{-3/2} + (C_{44}+\alpha)^{-3/2}],$$

$$B = \varrho^{3/2}[(C_{44})^{3/2} + \{C_{44}+\tfrac{1}{2}\,(\alpha-\beta)\}^{-3/2} + \{C_{44}+\tfrac{1}{2}\,(\alpha+\beta)\}^{-3/2}],$$

$$C = \varrho^{3/2}[2\{C_{44}+\tfrac{1}{3}\,(\alpha-\beta)\}^{-3/2} + \{C_{44}+\tfrac{1}{3}\,(\alpha+2\,\beta)\}^{-3/2}],$$

$$D = \varrho^{3/2}[(C_{44})^{-3/2} + \{C_{44}+\tfrac{1}{2}\alpha+\tfrac{1}{10}\,(9\,\alpha^2+16\,\beta^2)^{1/2}\}^{-3/2} + \{C_{44}+\tfrac{1}{2}\alpha-\tfrac{1}{10}\,(9\,\alpha^2+16\,\beta^2)^{1/2}\}^{-3/2}],$$

$$
\begin{aligned}
E = \varrho^{3/2}\big[&\{C_{44}+\tfrac{1}{6}\,(\alpha-\beta)\}^{-3/2} + \{C_{44}+\tfrac{1}{12}\,(5\,\alpha+\beta) + \tfrac{1}{12}\,(9\,\alpha^2+33\,\beta^2-6\,\alpha\beta)^{1/2}\}^{-3/2} \\
&+ \{C_{44}+\tfrac{1}{12}\,(5\,\alpha+\beta) - \tfrac{1}{12}\,(9\,\alpha^2+33\,\beta^2-6\,\alpha\beta)^{1/2}\}^{-3/2}\big],
\end{aligned}
$$

$$
\begin{aligned}
F = \varrho^{3/2}\big[&\{C_{44}+\tfrac{4}{9}\,(\alpha-\beta)\}^{-3/2} + \{C_{44}+(\tfrac{1}{18})\,(5\,\alpha+4\,\beta) + (\tfrac{1}{18})\,(9\,\alpha^2+48\,\beta^2+24\,\alpha\beta)^{1/2}\}^{-3/2} \\
&+ \{C_{44}+(\tfrac{1}{18})\,(5\,\alpha+4\,\beta) - (\tfrac{1}{18})\,(9\,\alpha^2+48\,\beta^2+24\,\alpha\beta)^{1/2}\}^{-3/2}\big],
\end{aligned}
$$

$$\alpha = C_{11} - C_{44}, \quad \beta = C_{12} + C_{44}.$$

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 Θ_1, Θ_2, Θ_3,...,Θ_8 corresponding to J_1, J_2, J_3,...J_8. It has been shown by BETTS et al.[7 a] that in case $\eta[=2\,C_{44}/(C_{11}-C_{12})]$ 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.

$$K_V = \tfrac{1}{9}(C_{11} + C_{22} + C_{33}) + \tfrac{2}{9}(C_{12} + C_{23} + C_{13}),$$
$$G_V = \tfrac{1}{15}(C_{11} + C_{22} + C_{33}) - \tfrac{1}{15}(C_{12} + C_{23} + C_{13}) + \tfrac{1}{5}(C_{44} + C_{55} + C_{66}).$$

$$(11)$$

REUSS [19] obtained, however, a different set of relations for K and G which are

$$(K_R)^{-1} = (S_{11} + S_{22} + S_{33}) + 2(S_{12} + S_{23} + S_{13}),$$
$$15(G_R)^{-1} = 4(S_{11} + S_{22} + S_{33}) - 4(S_{12} + S_{23} + S_{13}) + 3(S_{44} + S_{55} + S_{66})$$

$$(12)$$

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])

$$C_{11} = (S_{11} + S_{12})/(S_{11} - S_{12})(S_{11} + 2 S_{12}),$$
$$C_{12} = -S_{12}/(S_{11} - S_{12})(S_{11} + 2 S_{12}),$$
$$C_{44} = 1/S_{44},$$
$$S_{11} = (C_{11} + C_{12})/(C_{11} - C_{12})(C_{11} + 2 C_{12}),$$
$$S_{12} = -C_{12}/(C_{11} - C_{12})(C_{11} + 2 C_{12}),$$
$$S_{44} = 1/C_{44}.$$

$$(13)$$

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,

$$K_H = \tfrac{1}{2}(K_V + K_R),$$
$$G_H = \tfrac{1}{2}(G_V + G_R).$$

$$(14)$$

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

$$\bar{v}_s = (G_H/\varrho)^{1/2},$$
$$\bar{v}_l = [(K_H + \tfrac{4}{3} G_H)/\varrho]^{1/2}.$$

$$(15)$$

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.

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

$$(16)$$

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 Θ_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, δ, less than 20 percent, the approximation error, ξ, is less than 2 percent where these quantities are defined as

$$\delta = \frac{3[2 C_{44} - (C_{11} - C_{12})]^2}{12 C_{44}{}^2 + 38 C_{44}(C_{11} - C_{12}) + 3(C_{11} - C_{12})^2}, \quad (17)$$

$$\xi = (\bar{v}_m - v_m)/v_m. \quad (18)$$

The relationship between ξ and δ 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 [7a]. Although there are more than sixty semiconductors having cubic structure (cf. LAWSON and NIELSON [23]), the DEBYE temperatures have been reported here for only seventeen of them. This is due to the non availability of elastic and latice 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-

[18] W. VOIGT, Lehrbuch der Kristallphysik, B. G. Teubner, Leipzig 1928.
[19] A. REUSS, Z. angew. Math. Mech. **9**, 55 [1929].
[20] R. HILL, Proc. Phys. Soc., Lond. A **65**, 349 [1952].
[21] J. J. GILVARRY, 1956, Phys. Rev. **103**, 1700 [1956].

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

[22] C. KITTEL, Introduction to Solid State Physics, John Wiley & Sons, New York 1956.
[23] W. D. LAWSON and S. NIELSEN, Preparation of Single Crystals, Butterworths Scientific Publications, London 1958.

Material	Elastic Constants 10^{11} dynes/cm^2				Lattice Constant Å		Density gm/cm^3	
	C_{11}	C_{12}	C_{44}	Ref.	a_0	Ref.	ϱ	Ref.
C	94.90	15.10	52.10	a	3.566	a	3.51536	a
Si	16.56	6.386	7.953	a	5.4307	a	2.3283	a
Ge	12.88	4.825	6.705	a	5.657	a	5.3234	a
AlSb	8.94	4.43	4.15	a	6.1356	a	4.218	a
GaAs	11.88	5.38	5.94	b	5.5358	a	5.307	a
GaSb	8.85	4.04	4.32	a	6.095	a	5.619	a
InAs	8.329	4.526	3.959	c	6.058	a	5.872	d
InSb	6.717	3.665	3.018	a	6.4788	a	5.775	a
ZnS	10.79	7.22	4.12	a	5.406	a	4.079	a
ZnSe	8.10	4.88	4.41	e	5.667	a	5.420	a
ZnTe	7.13	4.07	3.12	e	6.101	a	5.720	a
CdTe	5.351	3.681	1.994	f	6.477	a	6.06	a
Mg$_2$Si	10.46	1.67	4.25	g	6.338	a	1.95	a
Mg$_2$Ge	10.43	1.41	4.30	g	6.378	a	3.086	a
PbS	12.70	2.98	2.48	h	5.92	h	6.6068	h
FeS$_2$	36.20	−4.40	10.40	i	5.41	j	5.035	d
PbTe	10.72	0.768	1.300	k	6.50	a	8.16	a

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

[a] Selected Constants relative to Semiconductors (edited by P. AIGRAIN and M. BALKANSKI), Pergamon Press, London 1961.
[b] T. B. BATEMAN, H. J. McSKIMIN, and J. M. WHELAN, J. Appl. Phys. **30**, 544 [1959].
[c] D. GERLICH, J. Appl. Phys. **34**, 2915 [1963].
[d] Calculated by Authors.
[e] D. BERLINCOURT, H. JAFFE, and L. R. SHIOZAWA, Phys. Rev. **129**, 1009 [1963].

[f] H. J. McSKIMIN and D. G. THOMAS, J. Appl. Phys. **33**, 56 [1962].
[g] R. D. REDIN, U. S. Gov. Res. Rep. **38**, 59 [1963].
[h] S. BHAGAVANTAM and T. S. RAO, Nature, Lond. **168**, 42 [1951].
[i] HUNTINGTON et al. [1].
[j] S. C. PRASAD and W. A. WOOSTER, Acta Cryst. **9**, 169 [1956].
[k] N. G. EINSPRUCH and R. T. MANNING, J. Acoust. Soc. Amer. **35**, 215 [1963].

pare the results obtained by various methods. Only the recent and more reliable data has been used in this work. The density of the substance has been calculated, wherever necessary, using the relation

$$\varrho = (M \, S)/(N \, a_0^3)$$

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, $S = 8$ for elemental and $S = 4$ for compound semiconductors.

Material	Anisotropy Factor η	DEBYE Temperature in °K							
		Θ_1	Θ_2	Θ_3	Θ_4	Θ_5	Θ_6	Θ_7	Θ_8
C	1.303	1995.0	2260.7	1894.4	1603.8	2014.8	2026.1	2033.9	1986.1
Si	1.733	573.7	558.2	576.8	555.9	568.5	581.6	569.6	575.4
Ge	1.663	343.6	336.2	359.4	325.6	348.5	358.3	368.5	346.8
AlSb	1.840	270.3	273.2	271.7	286.1	272.7	299.8	254.0	276.7
GaAs	1.827	312.5	386.1	345.4	309.7	330.7	314.5	351.9	324.2
GaSb	1.842	237.9	265.7	233.1	179.4	246.4	231.8	258.5	244.8
InAs	2.132	225.6	239.4	239.9	211.5	233.4	236.1	243.6	235.6
InSb	1.974	183.4	181.0	186.2	176.8	185.1	180.9	185.8	174.4
ZnS	2.308	293.7	298.2	299.4	297.2	303.9	304.3	300.3	303.3
ZnSe	2.739	251.5	248.0	247.4	241.3	245.7	246.7	244.8	245.9
ZnTe	2.039	201.3	214.3	200.1	198.8	206.1	210.7	198.3	207.1
CdTe	2.388	140.6	143.2	143.0	193.2	143.8	148.8	143.2	145.1
Mg$_2$Si	0.967	443.9	444.1	443.3	461.9	443.7	447.4	439.0	444.4
Mg$_2$Ge	0.953	352.8	362.1	352.8	358.7	327.1	353.8	351.2	353.0
PbS	0.510	206.4	197.5	209.5	234.3	216.0	212.1	205.3	210.5
FeS$_2$	0.512	556.9	561.4	562.5	569.7	566.0	563.2	561.1	562.4
PbTe	0.261	141.4	142.5	149.7	161.1	146.0	146.0	146.1	146.1

Table 2. DEBYE Temperature Using the Method of BETTS, BHATIA and WYMAN.

The parameters used in the calculation of DEBYE temperatures of cubic crystals are C_{11}, C_{12}, C_{44}, a_0, ϱ 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, $\Theta_1, \ldots, \Theta_8$, for each crystal obtained by the method of BETTS et al. [7a] have been presented in Table 2.

The values of the DEBYE temperatures obtained by VRHG approximation and HOUSTON's [6] approximation viz. Θ_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 $\Theta_2, \ldots, \Theta_8$, the accuracy is also quite comparable.

Material	HOUSTON's Approximation	VRHG Approximation	STEIG-MEIER's Approximation	S. C. S.*	A. I. P.**
C	1995	2167	—	2240	2240
Si	573,7	637	—	639	645
Ge	343.6	377.5	—	400	374
AlSb	270.3	290.3	292	370	—
GaAs	312.5	348.6	344	355	—
GaSb	237.9	267.5	265.5	250	—
InAs	225.6	246.4	262	270	—
InSb	183.4	205.6	202.5	170	205
ZnS	293.7	331.3	—	315	300
ZnSe	251.5	327.8	—	400	—
ZnTe	201.3	217.4	—	250	—
CdTe	140.6	159.2	—	200	—
Mg²Si	443.9	551.2	—	—	—
Mg₂Ge	352.8	441.4	—	—	—
PbS	206.4	233.5	—	—	194
FeS₂	556.9	717.7	—	—	645
PbTe	141.4	171.3	—	137	—

Table 3. Comparison of DEBYE Temperatures.

* Selected Constants Relative to Semi-conductors.
** 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 [1]) — the values quoted generally differed in the first or second decimal places. This may correspond to an error of about 1 percent in Θ_D value. It has also been found that very few authors presented density data along with the elastic constants while reporting calculation of DEBYE Θ using a particular method. This is important since a slight difference in ϱ 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 [8a] on the calculation of DEBYE Θ 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 Θ_D values is negligibly small, one should not forget that the Θ_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 Θ_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 Θ_4 value is always very much different from all other seven values. Also, for anisotropy factor $\eta > 2$, Θ_5, Θ_6, Θ_7 and Θ_8 are much closer to each other than Θ_1, Θ_2 and Θ_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 Θ_D values obtained by VRHG approximation and the experimental values taken from the American Institute of Physics Handbook [24] 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 [17b]. The values obtained by VRHG

[24] American Institute of Physics Handbook, Mc-Graw Hill, New York 1963.

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 Θ_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 Θ.

Spinwellen in dünnen ferromagnetischen Schichten

Von RAINER J. JELITTO *

Institut für Theoretische Physik der Universität München

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.

Von allen Modellen, welche der quantenmechanischen Beschreibung des ferromagnetischen Zustandes dienen, stellt nach wie vor das HEISENBERG-Modell[1] lokalisierter Spins den günstigsten Kompromiß zwischen der Forderung nach physikalischer Richtigkeit einerseits und den Erfordernissen mathematischer Einfachheit andererseits dar.

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[2] $T^{3/2}$-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[3,4]. Bei Rechnungen über das Flächengitter und

die lineare Kette kommt es zu Divergenzen, deren tiefliegende Ursachen im Falle des Flächengitters erst 1961 durch DÖRING[5] geklärt werden konnten.

Legt man den Untersuchungen ein allseitig unendlich ausgedehntes Kristallgitter zugrunde, so werden die Rechnungen durch die Translationsinvarianz des HAMILTON-Operators erheblich vereinfacht; allerdings begibt 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.
[1] W. HEISENBERG, Z. Phys. 49, 619 [1928].
[2] F. BLOCH, Z. Phys. 61, 206 [1930].
[3] S. FONER u. E. D. THOMPSON, J. Appl. Phys. 30, 229 [1959].

[4] B. E. ARGYLE, S. H. CHARAP u. E. W. PUGH, Phys. Rev. 132, 2051 [1963].
[5] W. DÖRING, Z. Naturforschg. 16 a, 1008 [1961].