

some CBED contrast, and must be from a medium-thick 200–300 Å region. The lattice image formed from this pattern shows a very marked departure from the hexagonal symmetry shown in the image of Fig. 11(a) which was obtained with a much reduced beam convergence (as in Fig. 11b) and from a thinner region of the sample. Fig. 10(a) shows an image composed of diamond-shaped cells which bear no obvious relationship to a real-space projection. This phenomenon has been reported in summary (Goodman, Moodie, Whitfield, Morton & Rossouw, 1982) but without showing the corresponding diffraction patterns from which the images were obtained. Examination of Fig. 10(b) shows that reciprocal space is largely filled with reflexion intensities, due to the high beam convergence, and that we are as much imaging individual reflexions as we are imaging superposed orders in the usual understanding of (parallel illumination) lattice imaging. The superposition of such an amount of angular information must be difficult to interpret except in terms of symmetry, and this is just an extreme example of the phenomenon often noted, that thick-crystal images are difficult to match against those computed, even when beam convergence is taken into the

calculation, to some approximation. Fig. 10(b) suggests that some of this difficulty must arise from an extreme sensitivity to the precise placement of both the condenser and the objective apertures, as well as to the fact that a substantial background of diffuse intensity fills the region remaining between diffraction orders. It is noted, however, that the crystal region is still substantially thinner than that used for Fig. 1 where there is a marked intensity fringe structure within each disc. It is well known, however, that angular phase modulation appears within the discs at an earlier stage of thickness than that required for intensity modulation.

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## X-ray Debye Temperature for Hexagonal Crystals

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### Abstract

With the Debye continuum model an analytical expression is derived for the X-ray Debye temperature ( $\theta_M$ ) of a hexagonal crystal in terms of the elastic constants and this expression is used to calculate  $\theta_M$  for hexagonal crystals of 41 elements and compounds. Calculated results by numerical integration are also presented for the X-ray Debye temperature perpendicular to the hexad axis,  $\theta_{\perp}$ , and that parallel to it,  $\theta_{\parallel}$ . The calculated results are compared with experimental values, wherever data are available. A correction factor for the effect of dispersion is determined from the experimental data.

### Introduction

The Debye–Waller factor is an important parameter in the description of a solid entering into the analysis of

numerous solid-state properties (Blackman, 1955; Maradudin, Montroll, Weiss & Ipatova, 1971; Willis & Pryor, 1975; Wertheim, 1968; Lipkin, 1961) including the scattering factors for X-rays, neutrons and electrons (both in electron diffraction and the incoherent scattering of conduction electrons) in addition to the recoilless fraction in Mössbauer experiments.

However, there is a scarcity of experimental data on Debye–Waller factors or equivalently X-ray Debye temperatures in the literature, particularly in the case of non-cubic crystals. This scarcity may be ascribed, at least in part, to the numerous difficulties in the collection and analysis of the appropriate data (Herbststein, 1961), which are compounded for non-cubic crystals by the fact that in such systems the Debye–Waller factors are anisotropic. In the analysis of results based on X-ray and neutron diffraction, corrections are necessary for thermal diffuse scattering. These are complicated by the fact that the thermal diffuse

scattering displays exceptional behaviour under Bragg peaks, itself peaking for X-rays (Zachariasen, 1969) and faster than sound neutrons. Furthermore, the interpretation of X-ray diffraction measurements is additionally complicated by the effect of Compton scattering, extinction, and anisotropic atomic scattering lengths. While determinations of Debye–Waller factors using Mössbauer measurements are not subject to the above difficulties, the number of isotopes suitable for such investigations is limited. Results based on Mössbauer measurements using a low concentration of a suitable isotope in a host lattice yield information regarding the lattice dynamical properties of an impurity atom in the host lattice, from the analysis of which the Debye–Waller factor of the host lattice can be obtained only by making questionable assumptions regarding the coupling of the impurity to the host lattice.

The Debye model has served as some sort of a ‘base’ for many solid-state investigations. However, it is known that it is inadequate for predicting X-ray Debye temperatures: in general it leads to values larger than those for actual solids. Hewat (1972) has proposed a model for calculating X-ray Debye temperatures in which acoustic modes are represented by sinusoidal dispersion relations. Treating any optical modes as continuations of acoustic modes, a reasonable approximation for simple compounds whose constituent atoms have similar masses, this results in X-ray Debye temperatures lower by a constant factor  $1/(2 \ln 2)^{1/2} \approx 0.85$  than those predicted by a dispersionless model. This constant 0.85 may be considered to be a sort of correction factor to allow for the dispersion.

In the present paper, using the Debye continuum model, we derive an analytical expression for the X-ray Debye temperature,  $\theta_M$ , for a hexagonal crystal in terms of the elastic constants and calculate  $\theta_M$  for 41 hexagonal crystals. Calculated results, by numerical integration, are also presented for the X-ray Debye temperature perpendicular to the hexad axis,  $\theta_{\perp}$ , and that parallel to it,  $\theta_{\parallel}$ . Wherever feasible, the calculated results are compared with experimental values. The correction factor for the effect of dispersion is determined from the experimental data.

### Theory

For a general harmonic crystal the temperature factor for the  $\kappa$ th atom in the unit cell is given by (Willis & Pryor, 1975):

$$T_{\kappa}(\mathbf{Q}) = \exp\left[-\frac{1}{2} \langle (\mathbf{Q} \cdot \mathbf{u}_{\kappa})^2 \rangle\right], \quad (1)$$

where  $\mathbf{u}_{\kappa}$  is the displacement of the  $\kappa$ th atom in the unit cell,  $\mathbf{Q}$  is the scattering vector,  $\mathbf{Q} = 4\pi (\sin \theta / \lambda) \cdot \mathbf{n}$ . For X-ray scattering,  $\theta$  being the Bragg angle,  $\lambda$  the wavelength of the X-rays and  $\mathbf{n}$  a unit normal to the scattering plane.

Since the scattering vector is time independent it may be removed from the average,

$$T_{\kappa}(\mathbf{Q}) = \exp\left(-\frac{1}{2} \mathbf{Q}^T \mathbf{B}_{\kappa} \mathbf{Q}\right), \quad (2)$$

where  $\mathbf{B}_{\kappa} = \langle \mathbf{u}_{\kappa} \mathbf{u}_{\kappa}^T \rangle$ . In general the  $\mathbf{B}_{\kappa}$  matrix has six independent components. However, for hexagonal crystals, symmetry requirements reduce this number to two. In an orthogonal basis with the  $z$  axis coinciding with the hexad direction, the  $\mathbf{B}_{\kappa}$  matrix may be written as (Willis & Pryor, 1975)

$$\mathbf{B}_{\kappa} = \begin{pmatrix} \langle u_a^2 \rangle & 0 & 0 \\ 0 & \langle u_a^2 \rangle & 0 \\ 0 & 0 & \langle u_c^2 \rangle \end{pmatrix},$$

where  $\langle u_a^2 \rangle$  is the mean-square displacement along a direction perpendicular to the hexad axis and  $\langle u_c^2 \rangle$  is the mean-square displacement parallel to the hexad axis.

It is often convenient to express the temperature factor in terms of an effective mean-square displacement,  $\langle u^2 \rangle_{\text{eff}}$ , for the direction of the scattering vector in question. For hexagonal crystals  $\langle u^2 \rangle_{\text{eff}}$  is given by:

$$\langle u^2 \rangle_{\text{eff}} = \langle u_a^2 \rangle \sin^2 \theta + \langle u_c^2 \rangle \cos^2 \theta, \quad (3)$$

where  $\theta$  is the angle between the hexad direction and the scattering vector,  $\mathbf{Q}_{\kappa}$ . Thus

$$T_{\kappa}(\mathbf{Q}) = \exp\left(-\frac{1}{2} Q^2 \langle u^2 \rangle_{\text{eff}}\right), \quad (4)$$

and from a knowledge of  $\langle u_a^2 \rangle$  and  $\langle u_c^2 \rangle$ , the temperature factor can be easily calculated for any scattering vector.

The  $\mathbf{B}_{\kappa}$  matrix can be calculated by applying Bose–Einstein statistics to a crystal’s normal modes

$$\mathbf{B}_{\kappa} = \frac{1}{m_{\kappa} N} \sum_{j\mathbf{q}} \frac{\hbar \mathbf{e}_{\kappa}(j\mathbf{q}) \mathbf{e}_{\kappa}^T(j\mathbf{q})}{\omega_{j\mathbf{q}}} \times \left[ \frac{1}{2} + \frac{1}{\exp(\hbar \omega_{j\mathbf{q}} / kT) - 1} \right],$$

where  $\omega_{j\mathbf{q}}$  is the angular frequency of a normal mode with wavevector  $\mathbf{q}$ ,  $\mathbf{e}_{\kappa}(j\mathbf{q})$  is the polarization vector of the normal mode  $\omega_{j\mathbf{q}}$  for the  $\kappa$ th atom in the unit cell, and  $T$  is the temperature of the lattice.

Although the Debye theory of lattice vibrations is a considerable simplification, experimental results are often expressed in terms of it because it leads to a single characteristic parameter, the Debye temperature, which varies relatively slowly with temperature.

For a true Debye solid, the Debye temperature appropriate for different thermodynamic averages would be the same, and temperature independent. However, for real solids, because of the different averages involved, each property involves a different Debye temperature which is temperature dependent (Salter, 1965). Moreover, for tensor properties such as

the mean-square displacement, the Debye temperatures involve tensors of the same rank.

In the Debye continuum model, dispersion is neglected and the frequency  $\omega$  is directly proportional to the wavevector  $q$ ,

$$\omega = v_0 q, \quad (5)$$

where  $v_0$  is a constant. For real solids, this is valid only for very small  $\omega$ . For the specific heat  $C_v$ , as  $T \rightarrow 0$  K, only low-energy modes contribute and the Debye approximation becomes exact, and thus the Debye temperature calculated from the elastic constants becomes equal to the calorimetric Debye temperature at 0 K. However, the average appropriate for the mean-square displacement matrix is such that all modes contribute even at absolute zero as a result of the zero-point energy contribution. Thus even in this limit, the Debye approximation is not exact. At high  $\omega$ , the dispersion curves for real solids show considerable departure from (5). Consequently, the X-ray Debye temperature calculated from the elastic constants will differ from the actual X-ray Debye temperature. We shall introduce a correction factor later on to allow for this difference.

For a hypothetical dispersionless crystal with hexagonal symmetry the value of the characteristic temperature is given in terms of the velocities of long-wavelength elastic waves,

$$\theta_M^{el} = \frac{h}{k} \left( \frac{3N}{4\pi V} \right)^{1/3} v_m, \quad (6)$$

where  $h$  is the Planck's constant,  $k$  is the Boltzmann constant,  $N/V$  is the number density of atoms and  $v_m$  is an average velocity. The values of  $v$  for  $\theta_{||}$ ,  $\theta_{\perp}$  and  $\theta$ , the equivalent isotropic Debye temperature, are given by  $v_{m||}$ ,  $v_{m\perp}$  and  $v_m$  respectively:

$$v_{m||}^2 = \left[ \int \sum_{i=1}^3 \frac{\cos^2 \theta_i(\Omega)}{v_i^2(\Omega)} \frac{d\Omega}{4\pi} \right]^{-1}$$

$$v_{m\perp}^2 = 2 \left[ \int \sum_{i=1}^3 \frac{\sin^2 \theta_i(\Omega)}{v_i^2(\Omega)} \frac{d\Omega}{4\pi} \right]^{-1}$$

and

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

where the sum on  $i$  is over the three elastic modes and  $\theta_i(\Omega)$  is the angle between the polarization vector of the elastic wave velocity  $v_i(\Omega)$  and the hexad axis,  $\Omega$  defining the direction of the wave vector.

The wave velocities and polarization vectors are the solutions of an eigenvalue problem (Musgrave, 1970),

$$(\Gamma - \lambda_i \mathbf{I}) \mathbf{e}_i = \mathbf{0}, \quad (7)$$

where  $\mathbf{e}_i$  is the polarization vector,  $\lambda_i$  is the eigenvalue for  $\mathbf{e}_i$  and is given by  $\lambda_i = \rho v_i^2(\Omega) - c_{44}$ ,  $\mathbf{I}$  is the identity matrix, and

$$\Gamma = \begin{pmatrix} n_1^2 A + \frac{1}{2} n_2^2 C & n_1 n_2 G & n_1 n_3 D \\ n_1 n_2 G & \frac{1}{2} n_1^2 C + n_2^2 A & n_2 n_3 D \\ n_1 n_3 D & n_2 n_3 D & n_3^2 H \end{pmatrix},$$

where

$$\begin{aligned} A &= c_{11} - c_{44}, & C &= c_{11} - c_{12} - 2c_{44}, \\ D &= c_{13} + c_{44}, & G &= \frac{1}{2}(c_{11} + c_{12}), \\ H &= c_{33} - c_{44}, \end{aligned}$$

$c_{ij}$ 's are the elastic constants of the crystal,  $\rho$  is the density and  $(n_1, n_2, n_3)$  a unit vector specifying the polar angle,  $\Omega$ .

Writing  $n^2 = n_3^2 = \cos^2 \theta$  and  $m = (1 - n^2)^{1/2}$ , we have

$$\lambda_1 = \frac{1}{2} m^2 C$$

$$\lambda_2 = \frac{1}{2} (m^2 A + n^2 H) + \left[ \frac{1}{4} (m^2 A + n^2 H)^2 + n^2 m^2 (D^2 - AH) \right]^{1/2}$$

$$\lambda_3 = \frac{1}{2} (m^2 A + n^2 H) - \left[ \frac{1}{4} (m^2 A + n^2 H)^2 + n^2 m^2 (D^2 - AH) \right]^{1/2}.$$

The corresponding eigenvectors for  $n_1 = 0$  are

$$\begin{aligned} \mathbf{e}_1 &= (1, 0, 0) \\ \mathbf{e}_2 &= (0, \cos \psi, -\sin \psi) \\ \mathbf{e}_3 &= (0, \sin \psi, \cos \psi), \end{aligned}$$

where

$$\tan \psi = \frac{m}{n} \left[ \frac{\lambda_3 - n^2(H - D)}{\lambda_3 - m^2(A - D)} \right].$$

Note that the only angular dependence is on  $\cos^2 \theta$  and  $\sin^2 \theta$ , so that it is not required to integrate on  $\psi$ . Thus

$$v_{m||}^2 = \left[ \int_0^{\pi/2} \left( \frac{\cos^2 \psi}{v_2^2} + \frac{\sin^2 \psi}{v_3^2} \right) \sin \theta d\theta \right]^{-1}$$

$$v_{m\perp}^2 = 2 \left[ \int_0^{\pi/2} \left( \frac{1}{v_1^2} + \frac{\sin^2 \psi}{v_2^2} + \frac{\cos^2 \psi}{v_3^2} \right) \times \sin \theta d\theta \right]^{-1}$$

$$v_m^2 = 3 \left[ \int_0^{\pi/2} \left( \frac{1}{v_1^2} + \frac{1}{v_2^2} + \frac{1}{v_3^2} \right) \sin \theta d\theta \right]^{-1}.$$

Table 1. *Calculated and experimental values of X-ray Debye temperatures in K*

The first row of values given for each element or compound gives the theoretical values. The experimental values are given in square brackets and those determined from neutron scattering and Mössbauer experiments are identified by (*N*) and (*M*) respectively. Experimental values without any identification are from X-ray experiments.

Solid	$\theta_{\perp}^{el}$	$\theta_{\parallel}^{el}$	$\theta_M^{el}$
Be	1442.4	1538.9	1472.5
Mg	374.1	380.1	376.2
	[ 329 <sup>a</sup>	303 <sup>a</sup>	315 <sup>b</sup> ]
Zn	365.7	269.7	323.3
	[ 317 + 35 <sup>c</sup> ( <i>M</i> )	180 + 7 <sup>c</sup> ( <i>M</i> )	]
	- 25	- 6	
		215 <sup>d</sup> ( <i>M</i> )	
Cd	223.8	169.4	200.3
	[ 166 <sup>a</sup>	97 <sup>a</sup>	]
Tl-1	70.5	95.5	76.6
Tl-2	70.3	96.2	76.5
Se	367.9	376.2	370.6
Y	249.4	252.6	250.5
Graphite	1338.2	290.8	481.5
	[ 1300 + 210 <sup>e</sup> ( <i>N</i> )	670 + 100 <sup>e</sup> ( <i>N</i> )	]
	- 110	- 70	
Ti	395.8	435.0	407.6
			270 ± 30 <sup>f</sup>
			350 ± 40 <sup>g</sup> ( <i>M</i> ) ]
Zr	281.0	292.5	284.7
			243 <sup>h</sup> ]
Hf	244.3	253.7	247.3
	[ 192 ± 13 <sup>i</sup> ( <i>M</i> )	227 ± 10 <sup>i</sup> ( <i>M</i> )	]
Re	400.3	413.8	404.7
			291 ± 10 <sup>j</sup> ( <i>M</i> ) ]
Co	455.4	493.3	467.0
Ru	515.6	502.1	512.7
			350 <sup>b</sup> ]
Pr	150.6	160.7	153.8
Nd	157.2	164.6	159.6
Gd	173.9	177.3	175.0
Tb	175.4	179.2	176.6
			170 ± 11 <sup>k</sup> ( <i>M</i> ) ]
Dy	181.3	185.0	182.5
Ho	184.2	187.7	185.4
	[ 147 ± 9 <sup>l</sup>	147 ± 9 <sup>l</sup>	147 ± 9 <sup>l</sup> ]
Er	189.3	191.7	190.1
Lu	182.3	180.7	181.8
AgI	134.4	172.6	144.2
			119 <sup>m</sup> ]
BeO-1	1299.9	1309.2	1303.0
BeO-2	1275.5	1309.2	1286.4
			1120 <sup>n</sup> ( <i>N</i> )
			1199 <sup>o</sup> ( <i>N</i> )
			875 ± 13 <sup>p</sup> ( <i>N</i> ) ]
ZnO	429.9	437.2	432.3
ZnS	355.3	368.0	359.4
ZnTe	224.7	226.2	225.2
CdS	220.2	227.9	222.7
CdSe	182.1	190.6	184.8
MnAs	234.2	318.4	254.4
SiC	1189.7	1197.9	1192.4
TbHo	200.3	206.3	202.2
SiO <sub>2</sub> *	589.0	548.1	574.4
CaMg <sub>2</sub>	368.3	371.1	369.2
Cd <sub>2</sub> Mg	165.1	161.6	163.9
MgZn <sub>2</sub>	312.9	328.8	317.9
TiB <sub>2</sub>	1033.7	1005.6	1024.0

Table 1. (*cont.*)

Solid	$\theta_{\perp}^{el}$	$\theta_{\parallel}^{el}$	$\theta_M^{el}$
CeF <sub>3</sub>	387.2	402.0	391.9
Cd <sub>3</sub> Mg	178.8	170.3	175.8
SmCo <sub>5</sub>	335.2	353.8	341.1
	[ 281 <sup>a</sup>	264 <sup>a</sup>	]
CsCuCl <sub>3</sub>	233.8	305.4	251.8

References: (*a*) Watanabe, Iwasaki & Ogawa (1971); (*b*) von Brill & Chopra (1962); (*c*) Kündig, Ando & Bömmett (1965); (*d*) Housley & Nussbaum (1965); (*e*) Ludsteck (1972), 300 to 1150 K; (*f*) Spreadborough & Christian (1959); (*g*) Moyzis, De Pasquali & Drickamer (1968); (*h*) Korsunskii, Genkin & Vigdorichuk (1971); (*i*) Boolchand, Robinson & Jha (1969), at 4 K; (*j*) Radeshütz & Langhoff (1976), at 9 K; (*k*) Enders, Weiss & Langhoff (1978), at 9 K; (*l*) Skelton (1969); (*m*) Burley (1964); (*n*) Pryor & Sabine (1964); (*o*) Sabine & Hogg (1968); (*p*) Kuleshov, Sadikov & Sokolova (1963); (*q*) Jennings & Chipman (1973), 300 to 1200 K.

\* Elastic constant data at 873 K.

The last integral can be evaluated analytically.\* The integrals for  $v_{m\parallel}^2$  and  $v_{m\perp}^2$  are not amenable to analytical evaluation.

### Data

The majority of experimental data on Debye-Waller factors for hexagonal crystals are from measurements at room temperature. Thus the Debye temperatures were calculated at room temperature to facilitate the comparison with experimental values. In the quasi-harmonic theory the appropriate elastic constants for this purpose are those at room temperature (Boyle & Hall, 1962), and thus room-temperature elastic constants were used. The experimental elastic constants employed in the calculations were taken from the compilation of Hearmon (1979). For Tl and BeO, two sets of elastic constants have been reported, which differ from each other and appear to have the same sort of accuracy; calculations were carried out for both sets and these are represented by Tl-1 and Tl-2, and BeO-1 and BeO-2 in Table 1. The density was taken from standard sources (Gray, 1972; Weast, 1978).

For calculating  $\theta_M$ , the analytical expression mentioned in the previous section was used, but for  $\theta_{\perp}$  and  $\theta_{\parallel}$ , numerical integration had to be used. The results are shown in Table 1 and, where data are available, compared with experimental X-ray Debye temperatures. The experimental values determined from neutron scattering and Mössbauer experiments are identified by (*N*) and (*M*) respectively.

\* The analytical solution has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38031 (3 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. Values of the ratio  $\theta(\text{expt.})/\theta^{\text{el}}$ 

Solid	$\theta_{\perp}(\text{expt.})/\theta_{\perp}^{\text{el}}$	$\theta_{\parallel}(\text{expt.})/\theta_{\parallel}^{\text{el}}$	$\theta_{\text{M}}(\text{expt.})/\theta_{\text{M}}^{\text{el}}$
Mg	0.879	0.797	0.837
Zn	0.867	0.667, 0.797	
Cd	0.742	0.573	
Graphite	0.971*	2.30*	
Ti			0.662, 0.859
Zr			0.854
Hf	0.786	0.895	
Re			0.719
Ru			0.683
Tb			0.963
Ho	0.798	0.783	0.793
AgI			0.825
BeO			0.865, 0.926, 0.676*
SmCO <sub>3</sub>	0.839	0.746	

\* Not used in taking the average.

### Discussion

It will be noticed from Table 1 that the experimental values of X-ray Debye temperatures are lower than the corresponding theoretical ones obtained from the elastic constants. The only exception to this behaviour is for graphite. As noted in the *Introduction*, an approximate theoretical model suggests a correction factor of 0.85 by which  $\theta_{\text{M}}$  calculated from the Debye theory should be multiplied to allow for the dispersion. Here we shall determine this correction factor from the experimental data. In Table 2 we show the ratio  $\theta(\text{expt.})/\theta^{\text{el}}$  for cases for which experimental values are available.

There are considerable uncertainties in the experimental values of the X-ray Debye temperature, as can be seen from the example of cases where two or more experimental values are available for the same solid. In view of this, we have obtained the correction factor by taking a global mean of all the ratios, except those for graphite and one of the values for BeO which is in serious disagreement with the other two values for this compound. The global mean is  $0.80 \pm 0.09$ . This is in fair accord with the theoretical estimate. The theoretical values for  $\theta$  for substances for which there are no experimental data can serve two purposes. If and when experimental data become available for these substances, the listed theoretical values could be used to obtain the correction factor. Also, these values multiplied by 0.80 will provide a good estimate for  $\theta$  for actual crystals. The exceptional behavior of graphite appears to be due to its high anisotropy.

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