Effects of lattice dispersion and elastic anisotropy on the thermal properties of bcc metals

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Abstract. Two new parameters which take into account the effects of elastic anisotropy and phonon dispersion on lattice specific heat in the case of sodium and potassium have been evaluated. A new graded mesh method which uses a 162-direction approximation in (1/16) part of the Brillouin Zone (BZ) has been considered to evaluate the two parameters.

1. Introduction

The fundamental lattice dynamical models and their application to the study of the thermophysical properties of crystalline solids have been discussed in literature (Joshi and Rajgopal 1968; Rao 1979; Wallace 1972; Maradudin *et al* 1963). In the lattice dynamical model of Debye (1912), the medium is assumed to be dispersionless and that the crystal is elastically isotropic. A further assumption of the model is that the actual Brillouin zone is replaced by a sphere. The experimental neutron diffraction data (Bacon 1962; Dolling and Woods 1965) provided accurate information regarding the phonon dispersion relations and established the superiority of Born-Von-Karman (BVK) model (Blackman 1935, 1937).

An excellent review of Blackman's work on $\theta - T$ anomaly of two-dimensional and three-dimensional lattices has been given by Delaunay (1956) and Seitz (1940). The anomalous behaviour of $\theta -- T$ curves gives a qualitative indication of the contribution of the combined effect of dispersion and anisotropy to the lattice specific heat of crystals.

It has become customary to present the low temperature specific heat results in terms of a single Debye temperature θ (Wallace 1972; Cochran 1973). Recently, instead of a $\theta - T$ plot, a quantitative study has been made regarding the effect of dispersion and anisotropy on the specific heat of some bcc and fcc metals (Tolpadi 1979; Singh and Tolpadi 1983).

In the present investigation a 162-direction approximation has been used in (1/16) part of the BZ for calculating the phonon frequencies by employing a nine-parameter lattice dynamical model of some bcc metals. The same 162-direction approximation has been used to develop a generalized Debye model of cubic crystals. This has enabled us to determine quantitatively both the effects of lattice dispersion and

anisotropy on the thermal properties of crystals. The effects of both lattice dispersion and anisotropy on the specific heat and Debye-Waller factor of some fcc crystals have been recently reported (Mohapatra and Tolpadi 1987).

Two-dimensionless parameters α_d and β_a which consider the effect of lattice dispersion and anisotropy respectively are defined as

$$\alpha_d = (C_{VM} - C_{VD})/C_{VM}, \tag{1a}$$

$$\beta_a = (C_{VD} - C_{V\theta})/C_{VM}, \tag{1b}$$

where C_{VM} is the model specific heat which includes the effect of both phonon dispersion and lattice anisotropy of the crystal. C_{VD} is the modified Debye specific heat which takes into account lattice anisotropy but excludes the effect of phonon dispersion. $C_{V\theta}$ is the single parameter Debye specific heat which neglects the effect of both lattice anisotropy and phonon dispersion in the crystal. These parameters α_d and β_a have been calculated in the case of Na and K.

2. Lattice dynamical model

A nine-parameter lattice dynamical model has been developed by considering a modified form of angular force to investigate the thermal properties of crystals in the present study. The modified angular force used here is different from the models of Clark, Gazis and Wallis (CGW) (Clark *et al* 1964) and Delaunay (DAF) (1956).

In the present study the angular force is assumed to be proportional to the change of the angle in the equilibrium plane of the triangles formed by the three atoms. The equilibrium plane BAC of the three atoms A, B, C of the bcc crystal is given in figure 1. If S_a, S_b, S_c are the displacements of the three atoms from their equilibrium positions of the lattice, the change in the angle ϕ in the equilibrium plane BAC due to these displacements is given by

$$\delta\phi = \frac{(P_B \cdot n_{A,B})n_{A,B}}{R_{A,B}} + \frac{(P_C \cdot n_{A,C})n_{A,C}}{R_{A,C}} \cdot, \tag{2}$$
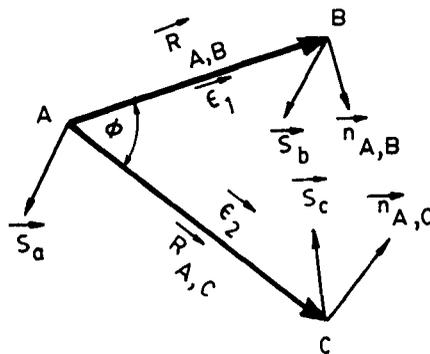

Figure 1. Angular force interaction with reference to a given set of three atoms A, B, C in case of bcc metal.

where $\mathbf{P}_B = \mathbf{S}_a - \mathbf{S}_b$, $\mathbf{P}_C = \mathbf{S}_a - \mathbf{S}_c$ and $\mathbf{n}_{A,B}$ and $\mathbf{n}_{A,C}$ are defined as unit vectors which are in the plane BAC and normal to the vectors $\mathbf{R}_{A,B}$ and $\mathbf{R}_{A,C}$ respectively.

Assuming $R_{A,B} = R_{A,C}$, the angular force on the reference atom A due to the change in the angle $\delta\phi$ is given by

$$\mathbf{F} = -\beta[(\mathbf{P}_C \cdot \mathbf{n}_{A,C})\mathbf{n}_{A,C} + (\mathbf{P}_B \cdot \mathbf{n}_{A,B})\mathbf{n}_{A,B}], \tag{3}$$

where β is the angular force constant.

In table 1, the types of angles $\phi_1, \phi_2 \ldots$ etc and the number of triangles considered in deriving the angular force expression for the bcc crystals are listed up to the fourth nearest neighbours. Using the data given in table 1, the total angular force on the reference atom A can be derived from (3).

Based on the present model, the frequency-determinant of the crystal has been derived by including the modified form of angular force up to the fourth nearest neighbours. The frequency determinant also includes the ion-ion central interaction upto fourth neighbours and the ion-electron interaction as given by Sarkar *et al* (1977). The secular equation of the bcc metals determining the frequencies v of the normal modes of vibration can be written as

$$|D_{ij} - 4\pi^2 M v^2(\mathbf{q})I| = 0, \tag{4}$$

where $i,j = 1, 2, 3$. I is the unit matrix of the order three, M is the mass of the atom $\mathbf{q}$ is the wave vector and D_{ij} are the matrix elements which include all the three interactions: ion-ion central, ion-ion angular and ion-electron interactions.

It is found that in the present model the expression for the bulk modulus in terms of elastic constants given by $(c_{11} + 2c_{12})/3$, contains angular force constants. Since the angles do not change when a crystal is subjected to uniform compression, the bulk modulus calculated by means of the static deformation method will not involve angular force constants (Singh and Dayal 1970; Born 1914; Wilson *et al* 1955; Herzberg 1962). To satisfy this criterion the following additional condition (5) involving the angular force constants is used in the present model.

$$\left(\frac{8}{3}\beta_1 + \frac{10}{3}\beta_2 + 8\beta_3 + \frac{88}{3}\beta_4\right) = 0. \tag{5}$$

Table 1. Data on the types of angles considered for the calculation of angular forces.

Neighbourhood	Angular force constant	Types of angles considered	Number of triangles
First	β_1	$\phi_1 = 70.52°$	12
		$\phi_2 = 109.47°$	12
Second	β_2	$\phi_1 = 90°$	8
Third	β_3	$\phi_2 = 90°$	12
Fourth	β_4	$\phi_1 = 35.097°$	24
		$\phi_2 = 129.52°$	12
		$\phi_3 = 144.9°$	24
		$\phi_4 = 50.48°$	12

3. Evaluation of specific heat

The specific heat of cubic crystals has been investigated by many workers earlier (Tripathi and Behari 1971; Behari and Tripathi 1970; Gupta and Tripathi 1971; Sharma and Awasthi 1979; Shukla and Cavalheiro 1973; Ramamurthy and Satish Kumar 1984) by calculating the phonon frequencies in (1/48) part of the BZ and applying Blackman's sampling techniques (Blackman 1935, 1937). At low temperature this method did not reproduce satisfactory results. Singh and Tolpadi (1983) and Mehrotra (1979) had suggested a graded mesh method which uses a 91-direction approximation in (1/16) part of the BZ. It was found that this method did not give the correct values of very low temperature specific heat when $(T/\theta) \simeq 2 \cdot 0 \times 10^{-3}$. Therefore, in the present work, an accurate method of evaluating the BZ sums using a 162-direction approximation, which uses the phonon frequencies in (1/16) part of the BZ has been developed. The wave vectors in (1/16) part of the BZ are generated by varying θ and ϕ from 0 to $\pi/2$ and 0 to $\pi/4$ respectively. The expression for the lattice specific heat C_V can be written as

$$C_V = \frac{16R}{V_q} \int_0^{\pi/2} \sin\theta \, d\theta \int_0^{\pi/4} I(\theta, \phi) \, d\phi, \tag{6}$$

where V_q is the volume of the first BZ and

$$I(\theta, \phi) = \sum_j \int_0^{q_z} x_{qj}^2 \frac{\exp(x_{qj})}{[\exp(x_{qj}) - 1]^2} q^2 \, dq. \tag{7}$$

In (7) $x_{qj} = h v_{qj}/kT$, $q_z(\theta, \phi)$ represents the zone boundary value of the wave vector in a given direction (θ, ϕ) and the summation in (7) is to be carried over all the three branches j.

In the present study phonon frequencies in (1/16) part of the BZ have been obtained from the frequency determinant given in (4). Using these results the model specific heat C_{VM}, which includes the effect of lattice dispersion and anisotropy, has been determined from (6) by using the numerical integration technique given in §4.

To determine C_{VD}, the modified Debye specific heat which includes lattice anisotropy but ignores the effect of dispersion on the lattice specific heat, a linear relationship between v_{qj} and q has been assumed i.e.

$$\mathbf{V}_j(\theta, \phi) = (v_{qj}/q)_{q\to 0}, \tag{8}$$

where $\mathbf{V}_j(\theta, \phi)$ is the wave velocity in a given direction (θ, ϕ). $\mathbf{V}_j(\theta, \phi)$ can be obtained from the frequency-determinant of the well-known classical elasticity theory (Reissland 1972).

Using the assumption given in (8) and changing the variable dq to dx_{qj} the function C_{VD} can be written as

$$C_{VD} = \frac{16R}{V_q} \int_0^{\pi/2} \sin\theta \, d\theta \int_0^{\pi/4} I'(\theta, \phi) \, d\phi \tag{9}$$

where

$$I'(\theta, \phi) = (kT/h)^3 \sum_j \frac{1}{V_j^3(\theta, \phi)} \int_0^{x_z} x_{qj}^4 \frac{\exp(x_{qj})}{[\exp(x_{qj} - 1]^2} \, dx_{qj}. \tag{10}$$

The specific heat C_{VD} depends on the number of directions chosen and the corresponding zone boundary frequencies in (1/16) part of the BZ. Hence it includes the effect of lattice anisotropy.

The limiting value of the Debye temperature θ_D (elastic) is used to calculate the single parameter lattice specific heat $C_{V\theta}$ (Kittel 1976). The value of θ_D is given by (Singh 1981)

$$\theta_D^3 = \frac{h}{k}(9V_q/16F_1), \tag{11}$$

where

$$F_1 = \int_0^{\pi/2} \sin \theta \, d\theta \int_0^{\pi/4} \Sigma_j \frac{1}{V_j^3(\theta, \phi)} \, d\phi. \tag{12}$$

4. Numerical computation

Before the phonon frequencies are calculated, it is necessary to know the numerical values of the force constants. There are nine parameters in the present model viz. $\alpha_1, \alpha_2, \alpha_3, \alpha_4, \beta_1, \beta_2, \beta_3, \beta_4$ and ak_e. $\alpha s'$ and $\beta s'$ are the central and angular force constants respectively. ak_e is the bulk modulus of the electron gas (Sarkar *et al* 1977). These have been calculated by using the known values of three elastic constants (Alexandrov and Ryzhova 1961; Marquardt and Trivisons 1965), angular force condition given in (5) and five experimental zone boundary phonon frequencies in the principal symmetry directions of the bcc metals Na and K (Woods *et al* 1962; Cowley *et al* 1966).

As the earlier methods (Singh and Tolpadi 1983; Mehrotra 1979) did not give the correct values of low temperature specific heat, a more accurate method of determining the thermal properties in the entire temperature range is introduced. This has been achieved by using a more accurate Gaussian-quadrature formula (Stroud and Secrest 1966; Demidovich and Maron 1981). In this method of numerical integration the interval between the limits of integration is divided into some unequal parts. The Gaussian-quadrature formula is given by

$$F = \int_a^b f(x) \, dx = \frac{b-a}{2} \sum_{i=1}^n A_i f(x_i), \tag{13}$$

where $x_i = \frac{1}{2}(b + a) + \frac{1}{2}(b - a)t_i$ $(i = 1, 2, 3, \ldots, n)$ and A_i and t_i are the coefficients given in table 2.

In the present calculation the wave vectors for computing the corresponding phonon frequencies are generated in (1/16) part of the BZ by varying θ and ϕ from 0 to $\pi/2$

Table 2. The coefficient A_i and t_i in Gaussian quadrature formula for 9, 16 and 18 intervals.

n	i	t_i	A_i
9	1; 9	∓ 0.96816024	0.08127439
	2; 8	∓ 0.83603110	0.18064816
	3; 7	∓ 0.61337143	0.2606107
	4; 6	∓ 0.32425342	0.31234708
	5	∓ 0.0	0.33023935
16	1; 16	∓ 0.98799252	0.02715246
	2; 15	∓ 0.93727340	0.06225352
	3; 14	∓ 0.84820658	0.09515851
	4; 13	∓ 0.72441773	0.12462897
	5; 12	∓ 0.57097217	0.1495959
	6; 11	∓ 0.39415134	0.16915652
	7; 10	∓ 0.20119409	0.18260341
	8; 9	∓ 0.0	0.18945061
18	1; 18	∓ 0.99156517	0.02161601
	2; 17	∓ 0.95582395	0.04971455
	3; 16	∓ 0.89260247	0.07642573
	4; 15	∓ 0.80370496	0.10094204
	5; 14	∓ 0.69168704	0.12255520
	6; 13	∓ 0.55977083	0.14064291
	7; 12	∓ 0.41175116	0.15468467
	8; 11	∓ 0.25188622	0.16427648
	9; 10	∓ 0.08477501	0.16914238

and 0 to $\pi/4$ respectively. We choose $(18 \times 9) = 162$ directions in (1/16) of the BZ where θ and ϕ are varied in eighteen and nine steps respectively by considering the 18-point and 9-point Gaussian-quadrature formulae. The integrals over θ and ϕ in (6) and (9) are evaluated by applying (13).

It is realized that in the evaluation of the BZ sums, the contribution of the various regions of the BZ to the given functions is dependent on the temperature. At very low temperature, particularly when $T/\theta < 6.3 \times 10^{-3}$, the lattice specific heat is almost entirely contributed by the low frequency excited phonons near the central part of the BZ as shown in figure 4. For this purpose instead of generating uniformly spaced wave vectors in each directions, we divide each BZ direction (θ, ϕ) from $q = 0$ to $q = q_z$ into four parts from (i) $q = 0$ to $q_1 = q_z/10$ (ii) $q = q_1$ to $q_2 = 3q_z/10$ (iii) $q = q_2$ to $q_3 = 6q_z/10$ (iv) $q = q_3$ to q_z. The BZ sum in (7) can be written as the sum of four parts given by

$$I(\theta, \phi) = \sum_{i=1}^{4} F_i(q_i),$$
(14)

where

$$F_i(q_i) = \sum_{j=1}^{3} \sum_{n=1}^{16} f(q_{ijn}),$$

j and n refer to the summations over the three branches and the relevant subzones respectively.

Thus in all (162 × 16) = 2592 wave vectors are generated in each of the four subzones in (1/16) of the BZ. Therefore according to the above scheme a total (2592 × 4 × 16) = 165,888 wave vectors are generated in the entire BZ. The zone boundary values q in the four subzones áre in the ratio 1/10:3/10:6/10:1. It may therefore be noted that according to this graded mesh method, the volumes of the four subzones lying between $q = 0$ to $q_z/10$ (subzone I) $q = q_z/10$ to $q = 3q_z/10$ (subzone II), $q = 3q_z/10$ to $q = 6q_z/10$ (subzone III) $q = 6q_z/10$ to q_z (subzone IV) are in the ratio 1:8:207:784. The actual numerical computation using Gaussian-quadrature formula and the present choice of graded mesh gives accurate value of specific heat even at extremely low temperature $(T/\theta \simeq 2 \cdot 0 \times 10^{-3})$.

5. Results and discussion

In the present investigation, the numerical computation technique described in §4 is used to calculate the thermal properties of bcc metals. Appropriate computer programs have been developed tc calculate the force constants, phonon frequencies, the Debye temperature θ_D, model specific heat C_{VM}, modified Debye specific heat C_{VD}, the single parameter Debye specific heat $C_{V\theta}$, and the parameter α_d and β_a cf the two bcc metals potassium and sodium.

The calculated model specific heat C_{VM}, by using the graded mesh method and the phonon dispersion relations in the symmetry directions show very good agreement with the experimental results (Gray 1972; Woods *et al* 1962; Cowley *et al* 1966)

Table 3 gives the Debye temperature data for some bcc metals. It is seen that the calculated values of θ agree with the experimentally determined calorimetric Debye temperature θ_C (Gray 1972; Filby and Martin 1965; Clusius and Franzsine 1958).

The dispersion parameter α_d and the elastic anisotropy parameter β_a defined in (1) are calculated from the computed values of C_{VM}, C_{VD} and $C_{V\theta}$. The specific heat $C_{V\theta}$ is obtained from the calculated value of elastic Debye temperature θ_D. The temperature variation of α_d and β_a for Na and K is given in figure 2.

It is observed that α_d is positive and β_a is negative in the entire range of temperature. In the low temperature range when $(T/\theta < 6 \cdot 3 \times 10^{-3})$ the effect of elastic anisotropy and dispersion on lattice specific heat is $<0 \cdot 5\%$. In this low temperature range it is found that the Debye T^3 law is obeyed. In the higher temperature region with $(T/\theta) \geqslant 1 \cdot 0$, α_d and β_a are negligible so that C_V attains the classical value. Since α_d is

Table 3. Data on elastic (θ_D) and calorimetric (θ_c) Debye temperatures, maximum dispersion parameter (α_d) and minimum anisotropic parameter (β_a), of some bcc metals.

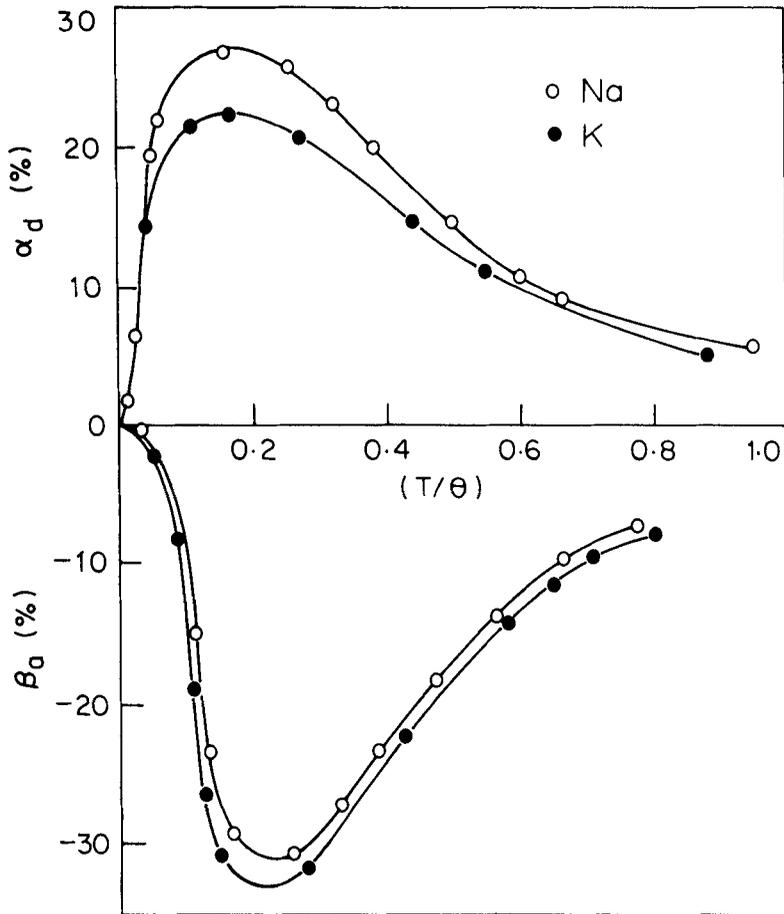| Metal	Anisotropy factor s	Debye temperature θ_D	θ_c	Temperature variation of α_d and β_a α_d	T/θ	β_a	T/θ
Rb	0·122	55·2	55·6	22·9	0·18	−35·5	0·18
K	0·131	90·9	90·6	22.1	0·17	−32·5	0·17
Na	0·134	157·8	158·0	26·6	0·16	−31·0	0·25
Fe	0·43	478·7	378·0	36·2	0.12	−12·0	0·21
W	1·0	383·5	467 0	37·4	0·13	−8·6	0·26

Figure 2. Temperature variation of the dispersion parameter (α_d) and anisotropic parameter (β_a) for Na and K.

positive and negligible in the low and high temperature regions, the temperature variation of α_d is expected to show a maximum in the intermediate temperature region. The maximum values of α_d in case of bcc metals are given in table 3 as a function of the elastic anisotropy factor $s = (c_{11} - c_{12})/2c_{44}$ (Delaunay 1956). α_d shows a maximum when $(T/\theta) \simeq 0.16$ in the case of Na and K.

The temperature variation of the elastic anisotropy parameter β_a given in figure 2 is found to be negative and negligible in the low and high temperature regions. Further β_a shows a minimum when $(T/\theta) \simeq 0.22$ for Na and K. The minimum values of β_a given in table 3 for bcc metals show that the magnitude of β_a decreases as anisotropy factor s increases. The minimum values of β_a vary in the range 8.6 to 35.5% while the corresponding variation in s is from 1 to 0.12.

To represent the departure from Debye criterion the temperature variation of the parameter $(\alpha_d + \beta_a)$ for Na and K. is plotted in figure 3. It is found that in case of Na and K, $(\alpha_d + \beta_a)$ is positive when (T/θ) varies from 0.01 to 0.12 and it is negative when $(T/\theta) > 0.12$. For a Debye solid $(\alpha_d + \beta_a)$ must be zero throughout the range of temperature. It is interesting to note that in the case of Na and K when $(T/\theta) \simeq 0.12$
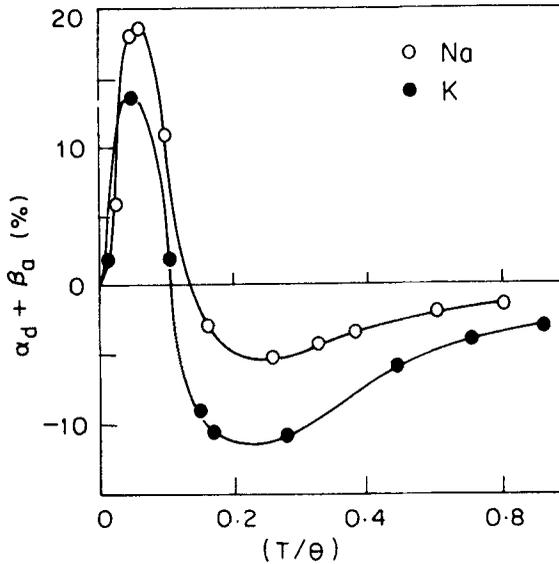
Figure 3. Temperature variation of $(\alpha_d + \beta_a)$ for Na and K.

the crystal behaves like a Debye solid. At this temperature the effect of lattice dispersion $(\alpha_d \simeq 25\%)$ and elastic anisotropy $(\beta_a \simeq -25\%)$ mutually cancel out. In the case of Na and K when $(T/\theta) \simeq 0{\cdot}06$ the combined effect of lattice dispersion and anisotropy is maximum.

The individual contribution to the specific heat C_{VM} from the four subzones is shown in figure 4 for Na. It is observed that when the temperature $(T/\theta = 6{\cdot}3 \times 10^{-3})$ the major contribution to C_{VM} is from the first subzone ($\simeq 95\%$). Therefore at extremely low temperature when the effect of dispersion and anisotropy is negligible the contribution to lattice specific heat is dominantly from the low frequency modes near the centre of the BZ.

At a higher temperature when $T/\theta \simeq 0{\cdot}06$ as pointed out earlier, the combined effect of lattice dispersion and anisotropy is large and the contributions to the specific heat from the first subzone are small. The contributions from the second and fourth zones are 30% while from the third zone the contribution is nearly 40%. Therefore when $T/\theta \simeq 0{\cdot}06$, the vibrational frequencies which gets thermally excited corresponding to the wave vectors in the range $q = 0{\cdot}1$ to $q = q_z$ are responsible for lattice anisotropy and dispersion. It is found that for potassium, the zone contributions to specific heat shows a similar trend.

6. Conclusion

In the present study a 162-direction approximation using a new graded mesh method in $(1/16)$ part of the BZ has been developed to accurately calculate the thermal properties of crystalline solids. In this graded mesh method the volumes of the four subzones of the BZ are in the ratio $1:8:207:784$. Two new parameters α_d and β_a which consider the effect of lattice dispersion and anisotropy on the specific heat has been
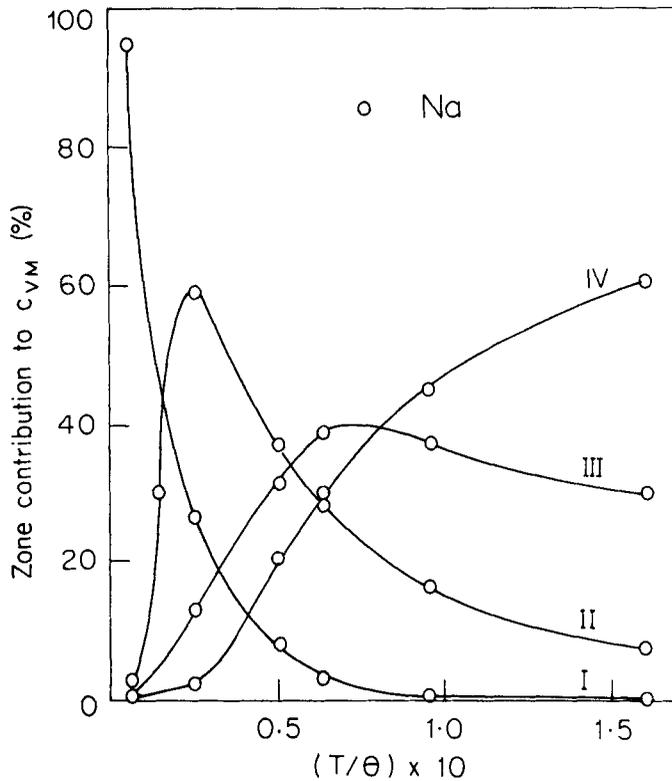
Figure 4. Temperature variation of the contribution to C_{VM} from the four subzones for Na.

calculated in Na and K. The temperature variation of the combined effect of dispersion and anisotropy $(\alpha_d + \beta_a)$ shows that it is maximum when $(T/\theta) \simeq 0.06$ and minimum when $(T/\theta) \simeq 0.2$ for both Na and K. Further in the region of the T^3 law, $(T/\theta \leqslant 6.3 \times 10^{-3})$ the contribution to the specific heat is from the first subzone. But it is found that when T/θ is in the range 0.04 to 0.4 the effect of lattice dispersion and anisotropy is large. In this range of temperature the frequencies corresponding to outer three subzones mainly contribute to the lattice specific heat.

Acknowledgement

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