Model for the lattice dynamics of hexagonal-close-packed metals

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The model we propose is an extension of Cheveau's approach to the hcp structure. This model satisfies the requirement of translational invariance as suggested by Lax, and is in equilibrium without recourse to external forces. In this, the short-range part is taken to be the first two terms in a Taylor's expansion of the potential energy. The first three nearest neighbors have been considered in obtaining the expressions for this contribution to the matrix elements. The long-range interaction has been accounted for on the lines of Krebs. Phonon dispersion relations along symmetry directions and the Θ-T curve have been plotted for magnesium and beryllium and compared with the available experimental results.

I. INTRODUCTION

The lattice vibrations of metallic crystals have been studied both theoretically and experimentally by many workers over the past several years.[1] The influence of the conduction electrons on the lattice vibrations was taken into account by de Launay[2] for the first time, who constructed a phenomenological model which includes explicitly the effect of a compressible but shear-free electron gas. The electron-gas models of Bhatia,[3] and Sharma and Joshi[4] have been successfully used in studying phonon dispersion relations, specific heats, and the Debye-Waller factor of a number of cubic metals. Gupta and Dayal,[5-7] Sharan and Bajpai,[8,9] and Verma and Upadhyay[10,11] incorporated phenomenologically the effect of conduction electrons on the lattice vibrations of hcp metals. Gupta and Dayal[5-7] extended Sharma and Joshi approach for studying the lattice dynamics of the hcp structure. They calculated the average strain set up in the atomic sphere owing to the thermal wave. In the case of metals whose axial ratio c/a is much greater than one, the replacement of the Wigner-Seitz polyhedron by an ellipsoid should be a better approximation. In view of this fact Sharan and Bajpai[8,9] modified the long-range matrix element of Gupta and Dayal. Later, Verma and Upadhyay[10,11] pointed out that the expression for the long-range part proposed by Sharan and Bajpai was incorrect. These authors suggested the correct expression.

These models suffer from three types of shortcomings. First, they violate the symmetry properties of a lattice in the sense that the secular equations in these theories are not invariant[12] with respect to a translation equal to a reciprocal-lattice vector, because of the nonperiodic contribution of the electron gas to the elements of the dynamical

matrix. Second, in these models the long-range matrix elements for the ions belonging to the non-basal planes were arbitrarily equated to zero. This is not true. In a physical model, ions belonging to the nonbasal planes contribute significantly to the matrix elements for the long-range part. Thirdly, all these models treat the electronic bulk modulus as a parameter. In some cases, e.g., in beryllium and yttrium, this is found to be negative. It seems to be unrealistic. Although the model of Krebs[13] satisfies the symmetry requirements, it suffers from a serious drawback of internal equilibrium. The derivative of the screened Coulomb interaction energy is not zero as it is for the short-range term. This necessitates an external force to be applied to maintain the system in equilibrium. Cheveau,[14] therefore, proposed a model for the cubic structure which not only satisfies the requirements of translational invariance but is also in equilibrium without recourse to external forces.

In view of the shortcomings inherent in the earlier models and the ideas put forward by Cheveau for the cubic metals, we thought it worthwhile to develop a model which is possibly free from these shortcomings.

II. PRESENT MODEL

In the present paper we have extended Cheveau's approach to the hexagonal close-packed structure. It is assumed that the forces on an ion may be regarded as arising from (a) a short-range (SR) central interaction $\phi(|\vec{r}|)$ between the ions, which is significant between the first, second, and third nearest neighbors, and (b) a long-range interaction (LR) steming from certain energies due to the presence of conduction electrons and their inter-

action with the ions.

Let the displacements of the central ion and its first-nearest-neighbor ions from their normal positions be $\vec{S}_0$ and $\vec{S}_{lmn}$. Then the total potential energy, when expanded in a Taylor series, is given by

$$\Phi = \sum_{lmn} \left\{ \frac{1}{r}\left(\frac{d\phi}{dr}\right)_{r=r_1} \left[\vec{r}^{\,0}_{lmn} \cdot (\vec{S}_{lmn} - \vec{S}_0) + \frac{1}{2} |\vec{S}_{lmn} - \vec{S}_0|^2 \right] \right.$$
$$\left. + \frac{1}{2}\left[\frac{1}{r}\frac{d}{dr}\left(\frac{1}{r}\frac{d\phi}{dr}\right) \right]_{r=r_1} [\vec{r}^{\,0}_{lmn} \cdot (\vec{S}_{lmn} - \vec{S}_0)]^2 \right\}.$$

$$(1)$$

$\vec{r}^{\,0}_{lmn}$ represents the position coordinates of neighboring atoms in equilibrium. The higher terms in the expansion of the Taylor series have been neglected. l, m, n represent the direction cosines of the line joining the central ion and a nearest neighbor. $\vec{r}_1$ is the nearest-neighbor distance. The summation in Eq. (1) extends over the first three nearest neighbors of the central ion at the origin. In this case the first derivative of the potential energy $(d\phi/dr)_{r=r_1}$ is not equated to zero. This is because our potential $\phi(|\vec{r}|)$ does not represent the entire potential determining the equilibrium distance $\vec{r}_1$.

The equation of motion of the ion at the origin is, therefore,

$$m\ddot{\vec{S}}_0 = -(\nabla_{S_0}\phi) + \vec{F}(0) . \qquad (2)$$

Here $\vec{F}(0)$ is the force exerted (on the ion at the origin) by the screened Coulomb interaction. The secular equation determining the angular frequencies ω of the normal modes of vibration in a crystal can be written as

$$|D(\vec{q}) - m\omega^2 I| = 0, \qquad (3)$$

where m is the mass of the ion in the lattice and I is the unitary matrix of the order 6×6. The dynamical matrix $D(\vec{q})$ is written as

$$D(\vec{q}) = \begin{pmatrix} A(\vec{q}) & B(\vec{q}) \\ B^*(\vec{q}) & A(\vec{q}) \end{pmatrix}, \qquad (4)$$

where $A(\vec{q})$ and $B(\vec{q})$ are 3×3 submatrices and $B^*(\vec{q})$ is the complex conjugate of $B(\vec{q})$. In the present approach the elements of the dynamical matrix $A_{ij}(\vec{q})$ and $B_{ij}(\vec{q})$ are expressed as the sum of two coupling coefficients:

$$A_{ij}(\vec{q}) = [A_{ij}(\vec{q})]^{SR} + [A_{ij}(\vec{q})]^{LR},$$
$$\qquad (5)$$
$$B_{ij}(\vec{q}) = [B_{ij}(\vec{q})]^{SR} + [B_{ij}(\vec{q})]^{LR}.$$

Superscripts SR and LR represent short-range and long-range interactions, respectively.

A. Short-range matrix elements

The expressions $[A_{ij}(\vec{q})]^{SR}$ and $[B_{ij}(\vec{q})]^{SR}$ have been estimated in view of Eq. (1). We have considered interaction between the central ion and its first three nearest neighbors. A unit cell of the hexagonal close-packed lattice contains two ions in it and its structure may be looked upon as being composed of two interpenetrating simple hexagonal lattices. Each ion of this lattice has six nearest neighbors at distances $(\frac{1}{4}c^2 + \frac{1}{3}a^2)^{1/2}$, six second neighbors at distances a, and six third neighbors at distances $(\frac{4}{3}a^2 + \frac{1}{4}c^2)^{1/2}$. Let α_1 and β_1 correspond to the expressions

$$\left(\frac{1}{r}\frac{d\phi}{dr}\right)_{r=r_1} \text{ and } \frac{1}{r_1}\left[\frac{d}{dr}\left(\frac{1}{r}\frac{d\phi}{dr}\right)\right]_{r=r_1}$$

of Eq. (1) for the first nearest neighbor. α_2, β_2 and α_3, β_3 are the similar terms for the second and third nearest neighbors, respectively. We have given in the appendix the expressions for $[A_{ij}(\vec{q})]^{SR}$ and $[B_{ij}(\vec{q})]^{SR}$.

B. Long-range matrix elements

This part arises from the Coulomb interaction between the ions of the lattice. The interaction is modified by the presence of conduction electrons, which give rise to screening. If the mutual separation between the two ions is $|\vec{r}|$, then the expression for the screened Coulomb potential is of the form

$$\phi(|\vec{r}|) \sim \frac{1}{|\vec{r}|} e^{-\lambda|\vec{r}|},$$

where λ is the screening parameter defined by

$$\lambda = \sigma\left(\frac{r_e}{a_0}\right)^{1/2} k_F$$

where r_e is the interelectronic spacing, k_F the Fermi wave vector, and σ is a parameter. According to Thomas and Fermi[15] the value of σ is 0.814 whereas according to Pines[16] it is 0.353. a_0 is the Bohr radius. Using the above expression for $\phi(|\vec{r}|)$ the following expressions for the long-range part of the matrix element have been obtained:

$$[A_{ij}(\vec{q})]^{LR} = A_p\left(\sum_{\vec{g}} \frac{(\vec{q}+\vec{g})_i(\vec{q}+\vec{g})_j}{|\vec{q}+\vec{g}|^2 + \lambda^2}\right.$$
$$\left. - \sum_{\vec{g}\neq 0} \frac{\vec{g}_i\vec{g}_j[1+\cos(\vec{g}\cdot\vec{r}_{12})]}{|\vec{g}|^2 + \lambda^2}\right), \qquad (6)$$

$$[B_{ij}(\vec{q})]^{LR} = A_p\left(\sum_{\vec{g}} \frac{(\vec{q}+\vec{g})_i(\vec{q}+\vec{g})_j}{|\vec{q}+\vec{g}|^2 + \lambda^2} e^{i(\vec{q}+\vec{g})\cdot\vec{r}_{12}}\right). \qquad (7)$$

Here A_p is a parameter, which depends upon the structure of the lattice. Its value is obtained in the long wavelength limit ($\vec{q} \to 0$). For hcp structure A_p is $(\sqrt{3}/4)a^2 c K_e \lambda^2$. Where K_e is the bulk modulus of the electron gas and $(\sqrt{3}/4)a^2 c$ is the atomic volume. The summation in Eqs. (6) and (7) extends over the reciprocal lattice vectors $\vec{g}$. $\vec{r}_{12}$ is the vector distance between the two ions in the unit cell.

Applying many-body perturbation theory, Langer and Vosko[17] were able to show that the screening parameter was a function of electron wave number $\vec{k}$. In view of the ideas put forward by these authors the modified screening parameter is given by

$$\lambda'^2 = \lambda^2 f(t),$$

where

$$f(t) = 0.5 + \frac{1 - t^2}{4t} \ln \left| \frac{1 + t}{1 - t} \right|$$

and

$$t = |\vec{q} + \vec{g}|/2k_F.$$

It was shown by Woll and Kohn[18] that if electron wave functions were treated to be Bloch type, then the free-electron expression included a function $G^2(x)$. Incorporating all these ideas in Eqs. (6) and (7), we write finally

$$[A_{ij}(\vec{q})]^{\text{LR}} = A_p \left(\sum \frac{(\vec{q} + \vec{g})_i (\vec{q} + \vec{g})_j G^2(x_1)}{|\vec{q} + \vec{g}|^2 + \lambda^2 f(t_1)} \right.$$
$$\left. - \sum_{\vec{g} \neq 0} \frac{\vec{g}_i \vec{g}_j G^2(x_2)[1 + \cos(\vec{g} \cdot \vec{r}_{12})]}{|\vec{g}|^2 + \lambda^2 f(t_2)} \right), \tag{8}$$

$$[B_{ij}(\vec{q})]^{\text{LR}} = A_p \sum \frac{(\vec{q} + \vec{g})_i (\vec{q} + \vec{g})_j G^2(x_1)}{|\vec{q} + \vec{g}|^2 + \lambda^2 f(t_1)} \exp[i(\vec{q} + \vec{g}) \cdot \vec{r}_{12}], \tag{9}$$

where

$$G(x) = 3(\sin x - x \cos x)/x^3$$

and

$$x_1 = (\vec{q} + \vec{g}) \cdot \vec{r}_e,$$
$$x_2 = \vec{g} \cdot \vec{r}_e,$$
$$t_1 = |\vec{q} + \vec{g}|/2k_F,$$
$$t_2 = |\vec{g}|/2k_F.$$

C. Elastic constants

In the long-wavelength limit ($\vec{q} \to 0$), the waves are effectively propagating as in a continuous medium. The long wavelength is obtained by expanding $D_{ij}(\vec{q})$ in powers of $\vec{q}$. The lowest nonvanishing terms are of the order of q^2 and in this limit we

can write the secular determinant as

$$\rho \omega^2 u_i = \sum_j [D_{ij}(\vec{q})] u_j, \tag{10}$$

where ρ is the electron density.

The easiest way to obtain the elastic constants expressed as a function of force constants is to put $\vec{q} \to 0$ in the dispersion relations. The acoustic modes in this region are linear. Therefore

$$\omega = 2\pi S |\vec{q}|, \tag{11}$$

where S is the velocity of sound such that

$$S = \sqrt{c'}/\rho . \tag{12}$$

Here c' is the elastic constant of the crystal. In the hexagonal-close-packed metals the determinant in Eq. (11) cannot be factorized everywhere and it is impossible to obtain all the five elastic constants. We have, therefore, obtained them using the standard long-wavelength procedure. By comparing Eq. (10) with the equation for the amplitude of the elastic waves,[19] we get the following expressions for the elastic constants in terms of the atomic force constants and the bulk modulus of the electron gas:

$$C_{11} - 2K_e = \frac{1}{2\sqrt{3}c} \left[3(X_1 + 3\beta_2 + 4X_2) + 4(\alpha_1 + 3\alpha_2 + 4\alpha_3) \right.$$
$$\left. - \frac{3(X_1 - 2X_2)^2}{6(\alpha_1 + \alpha_3) + 3(X_1 + X_2)} \right], \tag{13}$$

$$C_{12} - 2K_e = \frac{1}{2\sqrt{3}c} \left[(X_1 + 3\beta_2 + 4X_2) - 4(\alpha_1 + 3\alpha_2 + 4\alpha_3) \right.$$
$$\left. + \frac{3(X_1 - 2X_2)^2}{6(\alpha_1 + \alpha_3) + 3(X_1 + X_2)} \right], \tag{14}$$

$$C_{13} - 2K_e = \frac{\sqrt{3}c}{2a^2} \left[-2(\alpha_1 + \alpha_3) + (X_1 + X_2) \right], \tag{15}$$

$$C_{33} - 2K_e = \frac{1}{\sqrt{3}} \frac{c}{a^2} \left[3(\alpha_1 + \alpha_3) + \frac{9}{16} \gamma^2 (4X_1 + X_2) \right], \tag{16}$$

$$C_{44} = \frac{\sqrt{3}}{2} \frac{c}{a^2} \left[2(\alpha_1 + \alpha_3) + (X_1 + X_2) \right], \tag{17}$$

$$C_{44} = \frac{2}{\sqrt{3}c} \left[\alpha_1 + 3\alpha_2 + 4\alpha_3 + \frac{3}{4} \gamma^2 (X_1 + X_2) \right], \tag{18}$$

where

$$X_1 = \beta_1/(1 + \tfrac{3}{4}\gamma^2),$$
$$X_2 = \beta_3/(1 + \tfrac{3}{16}\gamma^2),$$

and

$$\gamma = c/a .$$

It is evident that the two expressions as given by Eqs. (17) and (18) have been obtained for the elastic constant C_{44}. In order that these may satisfy the

TABLE I. Input data for fixing the force constants.

Metal	Elastic constant C_{ij} (10^{11} dyn/cm^2)					K_e (10^{11} dyn/cm^2)	Lattice parameters (Å)		r_e (Å)	k_F (Å^{-1})	m (amu)	Experimental frequency (10^{12} Hz) $\Sigma_4[\text{TA}(\|)]$ at M
	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}		a	c				
Be	29.23	2.67	1.40	33.64	11.00	11.8967	2.2856	3.5832	0.9891	1.94	9.012	11.5
Mg	5.943	2.560	2.140	6.164	1.642	1.6346	3.2094	5.2105	1.4049	1.3704	24.312	3.71

condition for the lattice to be in equilibrium, the two values for C_{44} must be equal. This condition gives the following relationship

$$\alpha_2 + \alpha_3 = \tfrac{1}{6}(3\gamma^2 - 2)(\alpha_1 + \alpha_3). \tag{19}$$

D. Bulk modulus of the electron gas

As it has already been mentioned earlier, the bulk moduli of the electron gas for beryllium and magnesium have been calculated using the Virial theorem.[20] The required expression is given by

$$K_e = \kappa \left(\frac{1}{r_s} \frac{d^2\epsilon}{dr_s^2} - \frac{2}{r_s^2} \frac{d\epsilon}{dr_s} \right), \tag{20}$$

where κ is a constant whose value is 17.922×10^{22}. r_s is the radius parameter and ϵ is the total ground-state energy consisting of kinetic (ϵ_F), exchange (ϵ_{ex}) and correlation (ϵ_c) terms. Thus the total energy is given by[21-23]

$$\epsilon = \epsilon_F + \epsilon_{\text{ex}} + \epsilon_c, \tag{21}$$

where,

$$\epsilon_F = \frac{3}{5} \frac{\hbar^2}{2m^*} \left(\frac{3n}{8\pi} \right)^{1/3} n, \tag{22}$$

$$\epsilon_{\text{ex}} = -\frac{3}{4} \left(\frac{3}{\pi} \right)^{1/3} e^2 n^{1/3}, \tag{23}$$

and

$$\epsilon_c = -12.8527 + 0.5224 r_s + 1.6931 r_s^2 - 0.7928 r_s$$
$$+ 0.1628 r_s^4 - 0.0134 r_s^5, \tag{24}$$

and where m^* is the total effective mass and n is the density of the electron gas.

III. RESULTS

The values of electronic bulk modulus for Mg and Be as calculated from the expression (20) are given in Table I. The value of σ is taken to be 0.55 for Mg and 0.353 for Be.

The elastic constants have been measured by Smith and Arbogast[24] and Gold[25] in the case of beryllium and Slutsky and Garland[26] in the case of magnesium. Since the number of force constants is six, one additional condition is necessary to fix these force constants. For this purpose we have selected one known frequency ($\Sigma_4[\text{TA}(\|)]$) at the boundary of the Brillouin zone from the neutron dispersion data. The input data for fixing the force constants have been given in Table I. The calculated force constants for these metals are given in Table II. In the present paper all the elastic constants except C_{44} for beryllium are due to Smith and Arbogast.[24] The value 11.00×10^{11} dyn/cm^2 for C_{44} in the case of beryllium is found to give the best fit with the neutron-scattering data. The same value for C_{44} has been reported by Gold.[25]

The force constants have been used to calculate the phonon dispersion relations along [0001], [01$\bar{1}$0], and [11$\bar{2}$0] symmetry directions, which have been plotted in Figs. 1 and 3 along with the experimental points. For the computation of vibration spectra, the Brillouin zone is divided into a mesh of 1000 points, which reduce to 84 nonequivalent points (including the origin). All these points lie within the $\frac{1}{24}$th part of the Brillouin zone. When proper weightage is assigned to all these points we get 6000 frequencies. For the purpose of specific-heat computation with the help of Blackman's sampling technique, the frequency

TABLE II. Force constants (dyn/cm).

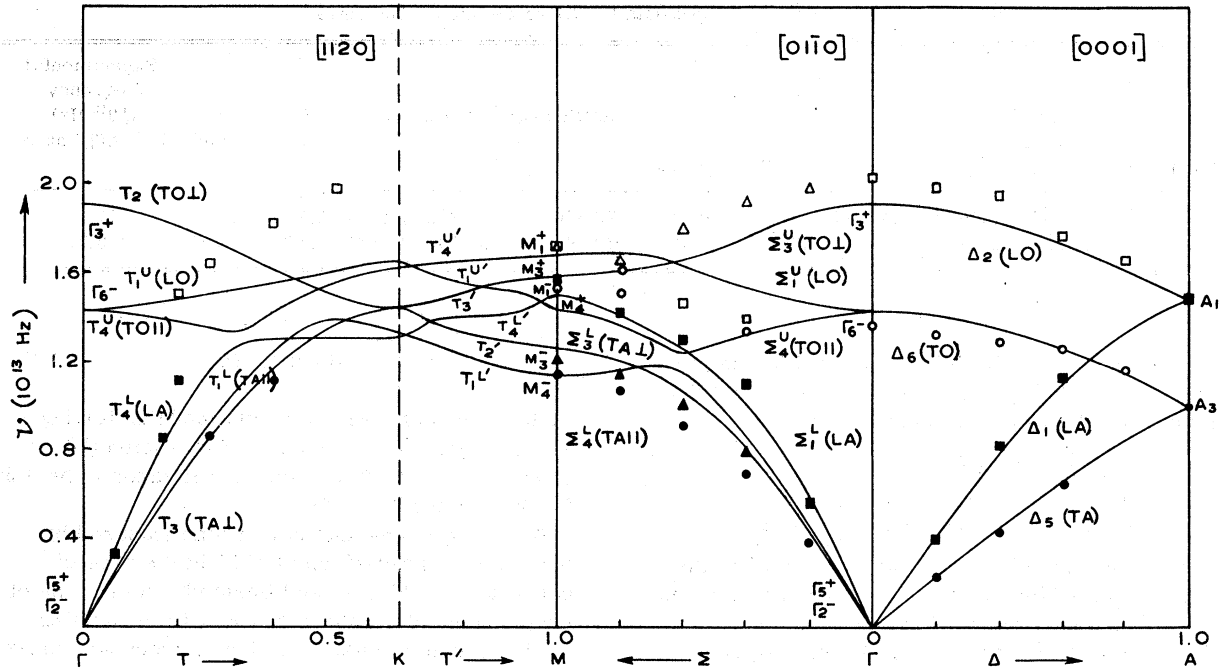| Metal | α_1 | α_2 | α_3 | $X_1 = \beta_1/(1 + \frac{3}{4}c^2/a^2)$ | β_2 | $X_2 = \beta_3/(1 + \frac{3}{16}c^2/a^2)$ |
| Be | 5981 | 4521 | 8069 | −971.6 | −4418.3 | −8613.4 |
| Mg | 340 | 317 | 1241 | 966.2 | 3139.4 | 380.9 |

FIG. 1. Dispersion curves for beryllium along [0001], [01$\bar{1}$0] and [11$\bar{2}$0] directions. Experimental points have also been shown for comparison.

spectrum is divided in steps of $\Delta\nu = 1.0$ THz in the case of beryllium and $\Delta\nu = 0.1$ THz in the case of magnesium. At very low temperatures, mesh becomes too coarse for accurate evaluation of specific heats on account of the dominant effect of the low-frequency end of the spectrum. The procedure gives very few frequencies in this region. The theoretical Θ-T curves are shown in Figs. 2 and 4 along with the experimental points.

IV. DISCUSSION

A. Beryllium

The phonon dispersion relations using inelastic scattering of slow neutrons have been measured by Schmunk et al.[27] and Schmunk.[28] The theoretical calculations on the phonon dispersion relations of Be have been made by Gupta and Dayal,[5] Sharan and Bajpai,[9] and Upadhyay and Verma[11] using

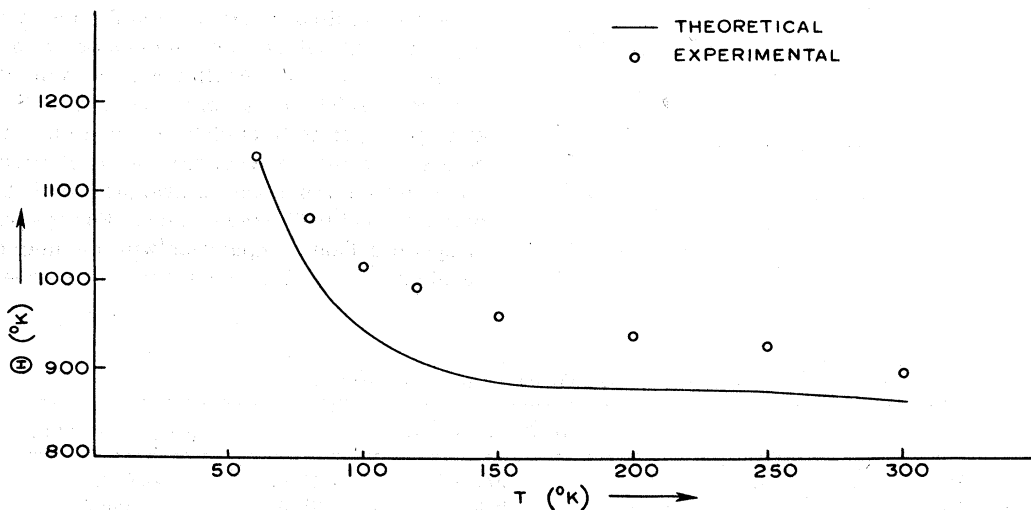FIG. 2. Θ-T curve for beryllium. Experimental points are shown for comparison.
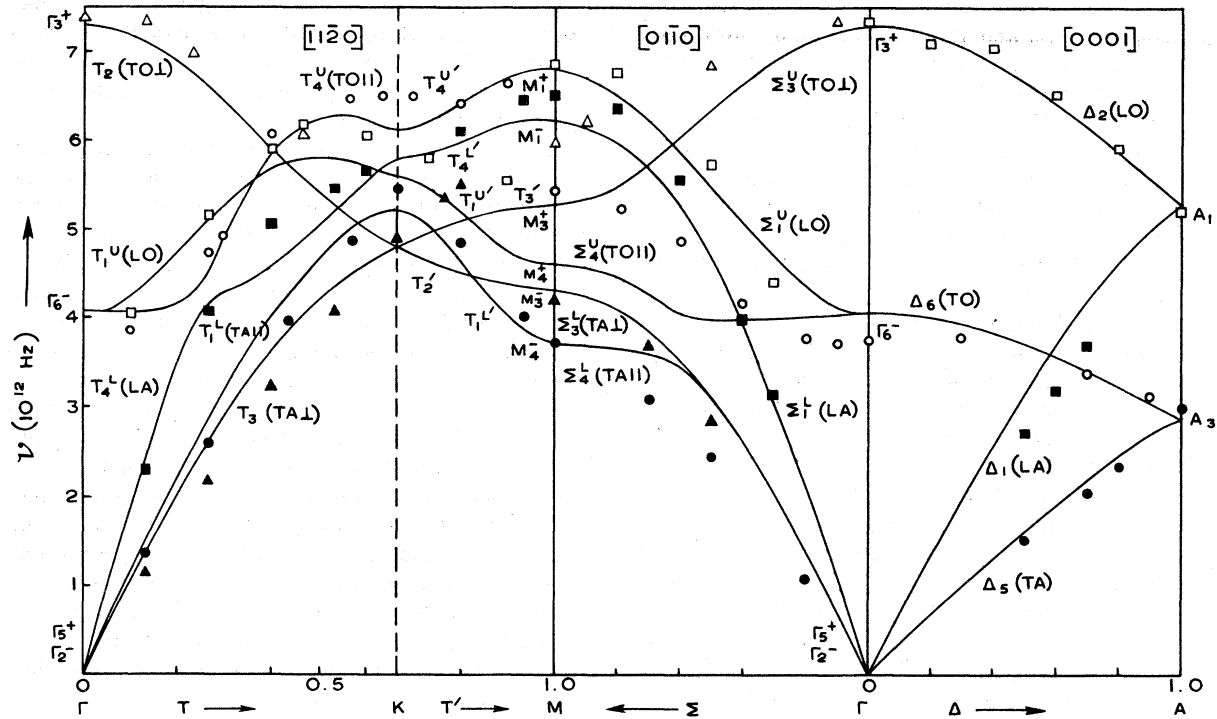
FIG. 3. Dispersion curves for magnesium. Experimental points have been plotted for comparison.

phenomenological models. The calculated results on the present model at the points M_1^-, M_1^+, M_3^+, M_4^+, A_1, and $\Gamma 3^+$ are 4.4%, 2.9%, 7.8%, 13.94%, 3.6%, and 6.8% lower, respectively, while at the points M_3^-, A_3, and $\Gamma 6^-$, they are 6.4%, 0.8%, and 5.2% higher than the experimental ones. In the [11$\bar{2}$0] direction the T_4(LO) branch deviates con-

siderably from the experimental phonon curve. The overall agreement between the present calculations and the experimental measurements on phonon dispersion relations for beryllium is better than those given by earlier workers who made the calculations only along [0001] and [01$\bar{1}$0] directions. Gupta and Dayal[5] and Sharan and Bajpai[9]
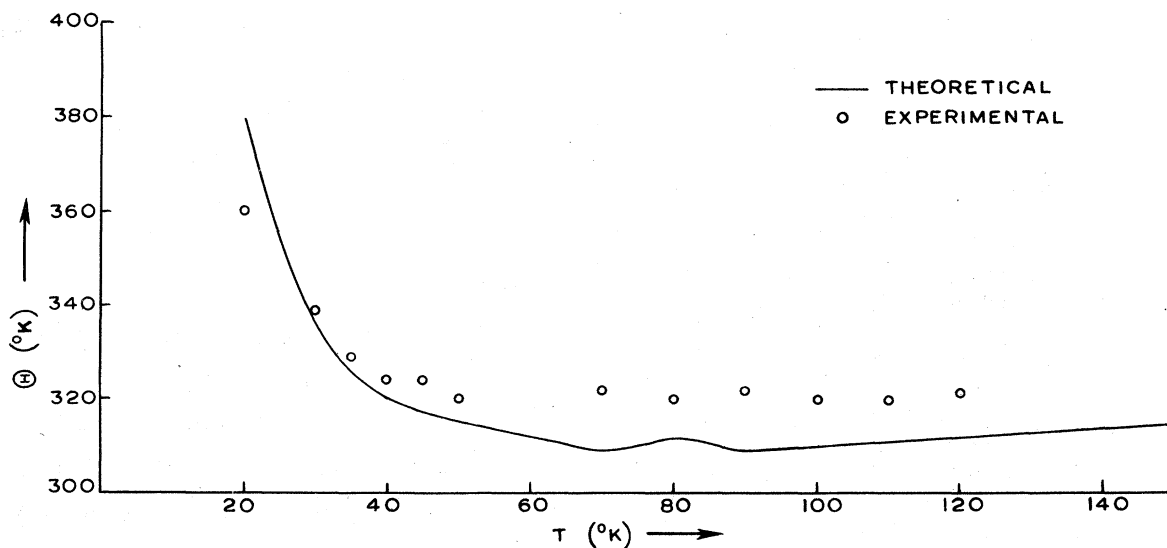

FIG. 4. Θ-T curve for magnesium. Experimental points have been shown for comparison.

have not calculated phonon frequencies corresponding to TA($\perp$) and TO($\perp$) modes along the [01$\bar{1}$0] direction. At some points their calculated results are 8%–12% higher than the observed frequencies. Upadhyay and Verma,[11] however, obtained good agreement between calculated and experimental frequencies. This is not surprising because an extensive fitting of the measured phonon frequencies was made by these authors. The theoretical results as given by these models are not shown in our figures.

The earliest measurements on the specific heats of beryllium from room temperature down to 10 K are due to Cristescu and Simon[29] and Hill and Smith.[30] There are three values available for γ_e (electronic-specific-heat coefficient). The first ($\gamma_e = 5.4 \times 10^{-5}$ cal/g-atom K^2) is due to Hill and Smith,[30] the second ($\gamma_e = 4.4 \times 10^{-5}$ cal/g-atom K^2) is due to Gmelin,[31] and the third ($\gamma_e = 4.05 \times 10^{-5}$ cal-g-atom K^2) is due to Ahlers.[32] The lattice contribution to the specific heat is calculated by subtracting the electronic specific heat $\gamma_e T$ from the experimental C_v. In Fig. 3, the calculated Θ-T curve is shown along with the experimental Θ values as obtained from the lattice specific heat of Hill and Smith.[30] Earlier such calculations were also done by Gupta and Dayal[6] and Rajput and Kushwaha.[33] Our results show slightly better agreement with the experimental data than those of these authors.

B. Magnesium

The earlier measurements on the phonon dispersion relations for magnesium are due to Collins[34] and Iyengar *et al.*[35] Subsequently the neutron inelastic-scattering measurements on the phonon frequencies for all the modes along [0001], [01$\bar{1}$0], and [11$\bar{2}$0] directions were performed by Pynn and Squires.[36] The theoretical calculations on the phonon dispersion relations for Mg have also been made by Gupta and Dayal,[7] Sharan and Bajpai,[9] and Upadhyay and Verma.[11] In all the cases, reasonably good agreements between the calculated and experimental phonon frequencies was obtained. As in the case of Be these authors have not made calculations along the [11$\bar{2}$0] symmetric direction. We have calculated phonon frequencies along the [11$\bar{2}$0] direction in addition to the common [0001] and [01$\bar{1}$0] directions. Our results compare very well with the observed frequencies.

The atomic specific heat in the case of magnesium at various temperature ranges has been measured by various workers.[37–42] For the calculation of experimental lattice specific heat we have taken the C_v values of Craig *et al.*[39] and the electronic specific-heat coefficient γ_e from the work

of Martin[42] ($\gamma_e = 2.927 \times 10^{-4}$ cal/g-atom K^2). The specific heat of Mg has also been calculated by Gupta and Dayal[7] and Rajput and Kushwaha.[33] The discrepancies between theoretical and experimental values for both the cases were within 3%–4%. Our results for Θ-T values show reasonably good agreement with the experimental values. Our theoretical results are almost comparable with the theoretical results of the earlier authors.

Recently Bertoni *et al.*[43] have emphasized the role of unpaired three-body forces in the theory of lattice dynamics of hcp metals. In the present model such forces have been introduced phenomenologically by considering terms like $(1/r)(d\phi/dr)$ in the Taylor expansion for potential energy of the crystal. The results on Debye characteristic temperature are also in fairly good agreement with the experimental results for both the metals. As mentioned earlier, the present model is free from most of the shortcomings of the earlier phenomenological models, and it is also microscopically sound in the sense that it explains the measured phonon dispersion relations satisfactorily. Besides this, it also explains the measured elastic constants.

ACKNOWLEDGMENT

APPENDIX

$$A_{11}^{SR} = 6(\alpha_1 + \alpha_3) + 3(X_1 + X_2) + \alpha_2(6 - 4C_1C_2 - 2C_{21})$$
$$+ \beta_2(3 - 2C_{21} - C_1C_2),$$

$$A_{22}^{SR} = 6(\alpha_1 + \alpha_3) + 3(X_1 + X_2) + \alpha_2(6 - 4C_1C_2 - 2C_{21})$$
$$+ 3\beta_2(1 - C_1C_2),$$

$$A_{33}^{SR} = 6(\alpha_1 + \alpha_3) + \tfrac{9}{8}\gamma^2(4X_1 + X_2)$$
$$+ \alpha_2(6 - 4C_1C_2 - 2C_{21}),$$

$$A_{12}^{SR} = \sqrt{3}\,\beta_2 S_1 S_2,$$

$$A_{13}^{SR} = 0,$$

$$A_{23}^{SR} = 0,$$

$$B_{11}^{SR} = -C_3[\alpha_1(2D_2 + 4C_1D_1^*) + \alpha_3(2D_4^* + 4C_{21}D_2)$$
$$+ 3X_1C_1D_1^* + 3X_2C_{21}D_2],$$

$$B_{22}^{SR} = -C_3[\alpha_1(2D_2 + 4C_1D_1^*) + \alpha_3(2D_4^* + 4C_{21}D_2)$$
$$+ X_1(C_1D_1^* + 2D_2) + X_2(C_{21}D_2 + 2D_4^*)],$$

$$B_{33}^{SR} = -C_3[\alpha_1(2D_2 + 4C_1D_1^*) + \alpha_3(2D_4^* + 4C_{21}D_2)$$
$$+ \tfrac{3}{2}\gamma^2 X_1(2C_1D_1^* + D_2) + \tfrac{3}{8}\gamma^2 X_2(2C_{21}D_2 + D_4^*)],$$

$$B_{12}^{SR} = i\sqrt{3}\,C_3(X_1 S_1 D_1^* - X_2 S_{21} D_2)\,,$$

$$B_{13}^{SR} = 3\gamma S_3(X_1 S_1 D_1^* + \tfrac{1}{2}X_2 S_{21} D_2)\,,$$

$$B_{23}^{SR} = i\sqrt{3}\,\gamma S_3[(C_1 D_1^* - D_2)X_1 - \tfrac{1}{2}X_2(C_{21}D_2 - D_4^*)]\,,$$

where

$$C_1 = \cos\tfrac{1}{2}a q_1,\quad C_2 = \cos\tfrac{1}{2}\sqrt{3}\,a q_2,\quad C_3 = \cos\tfrac{1}{2}c q_3,$$

$$S_1 = \sin\tfrac{1}{2}a q,\quad S_2 = \sin\tfrac{1}{2}\sqrt{3}\,a q_2,\quad S_3 = \sin\tfrac{1}{2}c q_3,$$

$$C_{21} = \cos a q,\quad S_{21} = \sin a q_1,\quad \gamma = c/a\,,$$

$$D_n = \exp(i a q_2 n/2\sqrt{3}\,),\quad i = \sqrt{-1}\,,$$

$$X_1 = \frac{\beta_1}{1+\tfrac{3}{4}\gamma^2},\quad X_2 = \frac{\beta_3}{1+\tfrac{3}{16}\gamma^2}\,.$$

D_n^* is the complex conjugate of D_n.

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