Phys. Soc. **14**, 402 (1969).

[31]B. W. Murray and J. D. McGervey, Phys. Rev. Lett. **24**, 9 (1970).

[32]A. Thompson, B. W. Murray, and S. Berko, Phys. Lett. A **37**, 461 (1971).

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Study of Phonon Dispersion in hcp Metals with Central Pair Potentials Representing Ion-Ion Interactions

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A phenomenological model for the study of the lattice dynamics of hcp metals has been developed by adding an approximate electron-ion-interaction term to a five-neighbor central pair potential. Application of the model to the four hcp solids Mg, Sc, Zr, and Ho leads to dispersion curves which generally present a good agreement with the corresponding experimental curves.

I. INTRODUCTION

Dispersion curves of a large number of hcp metals have been determined in recent years by the neutron-spectroscopic method. These curves provide the basic information for an understanding of the dynamics of the hcp lattice. The models generally employed for theoretical explanations of these curves are tensor-force (TF) model, the axially symmetric (AS) model, the modified axially symmetric (MAS) model, and a mixed-force (MF) model based on axially symmetric interactions and tensor forces acting among various neighbors.[1-5] Such models employ a large number of parameters and agreement with experimental curves, achieved by means of a least-squares fitting procedure, is often excellent. However, the fact that these models do not incorporate the metallic character of the solids makes them unsatisfactory from the theoretical point of view.

A relatively recent work on the lattice dynamics of the hcp system is that presented by King and Cutler[6] and is based on a model pseudopotential calculation. This work must be considered theoretically satisfactory, but the results of this study also show large deviations from experimental dispersion curves.

A serious question concerning theoretical models of lattice dynamics has been recently raised by Szigeti and co-workers.[7,8] These authors have shown from general considerations that the parameters of a theoretical model can be continuously varied over large ranges without affecting the order of agreement between the theory and the experiment. It has been pointed out that a unique set of values of the model parameters can in principle be determined if we also possess additional results on measurements of eigenvectors or those obtained by substitution of isotopes. In view of this work, the agreement with dispersion data can not be considered as enough proof of the validity of a theoretical model. However, until measurements on eigenvectors are available, the dispersion data will continue to remain the most dependable experimental results for theoretical workers in the field of lattice dynamics. In order to decide upon the superiority of one theoretical model over another, we can appeal to the principle of simplicity and the plausibility of the basic assumptions.

The main points of deviation from the lattice dynamics of cubic metals in the case of the hcp system are (i) the lower symmetry of this system and (ii) the range to which the ion-ion interactions are significant. The TF and AS models satisfy the symmetry conditions but have to employ force constants out to eighth neighbors for the best agreement with experimental dispersion curves. In view of the screening effect of the conduction electrons, it seems unlikely that the ion-ion interactions are significant out to such distant neighbors. In the work presented here we have tried to investigate this point phenomenologically using a force model that includes the effect of conduction electrons along the lines used by Sharma and Joshi[9] for cubic metals. The resulting electron-ion interaction does not satisfy the requirements of symmetry in the reciprocal space but can be considered satisfactory as far as numerical results are concerned. The ion-ion interactions have been derived from pair potentials. Such a representation of the ion-ion interactions has been discussed by Lahteenkorva,[10] but to reduce the number of parameters of his theory, so that they could be evaluated mainly from the expressions for the five elastic constants, he has used additional constraints and set some of the potential parameters equal to zero, resulting in a somewhat strange potential. We have avoided such artificial constraints by using an adequate number of vibration frequencies in addition to elastic constants in evaluating the model parameters. The resulting model can be considered as a modified axially symmetric model and has been used to study the lattice dynamics of a number of hcp metals for which experimental dispersion curves are available. The computed dispersion curves are found to agree closely with the experimental ones. In this paper we are reporting results on Mg, Sc, Zr, and Ho.

II. THEORY

Let us denote the position of the (l, κ)th atom by the vector $\vec{r}(l, \kappa)$ and its Cartesian components by $x_\alpha(l, \kappa)$, $\alpha = 1, 2, 3$. l is the integer triplet (l_1, l_2, l_3) and $\kappa = 1, 2$ is the basis index. The position of the (l', κ')th atom relative to the (l, κ)th will then be

$$\vec{r}(ll', \kappa\kappa') = \vec{r}(l', \kappa') - \vec{r}(l, \kappa) \;,$$

and the corresponding Cartesian coordinates are

$$x_\alpha(ll', \kappa\kappa') = x_\alpha(l', \kappa') - x_\alpha(l, \kappa) \;.$$

If Φ is the total-potential-energy function of the lattice, the frequencies ω of the normal modes of vibration in the harmonic approximation will be given by

$$\left| \mathrm{D}_{\alpha\beta}(\vec{\mathrm{k}}; \kappa\kappa') - m\omega^2 \delta_{\alpha\beta}\delta_{\kappa\kappa'} \right| = 0, \tag{1}$$

where m is the atomic mass, $\vec{\mathrm{k}}$ $(k = 2\pi/\lambda)$ the wave vector, $\delta_{\alpha\beta}$ and $\delta_{\kappa\kappa'}$ the Krönecker δ symbols, and

$$\mathrm{D}_{\alpha\beta}(\vec{\mathrm{k}}; \kappa\kappa') = \sum_{l'} \left(\frac{\partial^2 \Phi}{\partial x_\alpha(l, \kappa) \partial x_\beta(l', \kappa')} \right)_0 e^{i \vec{\mathrm{k}} \cdot \vec{\mathrm{r}}(ll', \kappa\kappa')} .$$

The subscript 0 after the large parentheses indicates that the expression inside has to be evaluated for the equilibrium configuration.

If Φ is built up of pair potentials $\phi(l' - l, \kappa\kappa')$, we can put

$$\mathrm{D}_{\alpha\beta}(\vec{\mathrm{k}}; \kappa\kappa') = - \sum_{\substack{l' \\ l, \kappa \neq l', \kappa'}}' \left(\frac{\partial^2 \phi(l' - l, \kappa\kappa')}{\partial x_\alpha(ll', \kappa\kappa') \, \partial x_\beta(ll', \kappa\kappa')} \right)_0 \times e^{i \vec{\mathrm{k}} \cdot \vec{\mathrm{r}}(ll', \kappa\kappa')} \;. \tag{2}$$

The coupling coefficients $\mathrm{D}_{\alpha\beta}(\vec{\mathrm{k}}; \kappa\kappa')$ can be broken up in parts corresponding to the different contributions to ϕ. In the case of metals, ϕ can be separated into two parts, one representing the ion-ion interaction ϕ^i and the other the ion-electron-ion interaction ϕ^e, i.e.,

$$\phi = \phi^i + \phi^e \;.$$

We assume the ion-ion interactions to extend up to fifth neighbors and denote the pair potential coupling the origin atom with a jth neighbor by ϕ^i_j. Thus the total ionic potential is split into five terms corresponding to the neighbors up to the fifth. Substitution of this potential in Eq. (2) expresses the coupling coefficients in terms of first and second r derivatives of ϕ^i_j. Let us put

$$\frac{d\phi^i_j}{dr_j} = A_j \quad \text{and} \quad \frac{d^2\phi^i_j}{dr_j^2} = B_j, \quad j = 1, 2, 3, 4, 5 \;. \tag{3}$$

Then

$$D^{(i)}_{\alpha\beta}(\vec{\mathrm{k}}; \kappa\kappa') = -\sum_j \sum_{\substack{j\text{th} \\ \text{neighbors}}} \left[B_j \frac{x_\alpha(j) x_\beta(j)}{r_j^2} + \frac{A_j}{r_j} \left(\delta_{\alpha\beta} - \frac{x_\alpha(j) x_\beta(j)}{r_j^2} \right) \right] e^{i \vec{\mathrm{k}} \cdot \vec{\mathrm{r}}(j)} \;. \tag{4}$$

The contribution of the ion-electron-ion interaction to the coupling coefficients can be calculated by classical considerations to a good approximation. One of the methods is that given by Sharma and Joshi.[9] This theory assumes that the adiabatic contribution of the conduction electrons to the ionic Hamiltonian is equal to the average strain energy of the electron gas arising due to the passage of lattice waves through it. To estimate this energy, the strain is averaged over the Wigner–Seitz sphere which approximates to the atomic polyhedron in cubic solids. In the hcp system the atomic polyhedron can be replaced by a suitable spheroid. The expression for the average strain over a spheroidal cell was first derived by Sharan and Bajpai.[11] These authors, however, made an algebraic error in the derivation which was later corrected by Verma and Upadhyaya.[12] The correct expressions for the electron-ion coupling coefficients thus obtained are given below:

$$\begin{aligned} \mathrm{D}^{(e)}_{\alpha\beta}(\vec{\mathrm{k}}; \kappa\kappa') &= K_e k_\alpha k_\beta \mathrm{G}^2 \Omega \;, \quad && \kappa = \kappa' \\ &= 0 \;, && \kappa \neq \kappa' \end{aligned} \tag{5}$$

where K_e is the bulk modulus of the electron gas, $\Omega = \frac{1}{4}\sqrt{3}\, a^2 c$ is the volume of the atomic polyhedron, and the function G (Verma and Upadhyaya[12]) is

$$G = \frac{3(\sin \lambda' k - \lambda' k \cos \lambda' k)}{(a_1^2 k_1^2 + a_2^2 k_2^2 + a_3^2 k_3^2)^{3/2}} \;, \tag{6}$$

$a_1 = a_2$, a_3 being the semiaxes of the atomic spheroid and λ' the largest projection along $\vec{\mathrm{k}}$ of the position vector of an infinitesimal element of the electron gas.

The lattice equilibrium is usually assumed to be determined by the ion-ion potential only. This assumption amounts to ignoring the pressure of the electron gas and introduces an error which is perhaps of minor importance. The equilibrium distances are functions of the two lattice parameters a and c. Therefore, the derivation of the equilibrium condition needs an auxiliary condition to connect the differentials of a and c. We have obtained this auxiliary condition by assuming the equilibrium volume of the unit cell to be stationary which requires

$$\frac{dc}{da} = -\frac{2c}{a} \quad . \tag{7}$$

Minimization of ϕ^i with the constraint (7) leads to the equilibrium condition

$$2\alpha_1 + \alpha_2\left(\frac{2}{3} - \frac{c^2}{a^2}\right) + \alpha_3\left(\frac{8}{3} - \frac{c^2}{a^2}\right) - \frac{4}{3}\,\frac{c^2}{a^2}\,\alpha_4 + 2\alpha_5\left(\frac{14}{3} - \frac{c^2}{a^2}\right) = 0 \quad , \tag{8}$$

which is similar to the one obtained by Collins[1] and can also be obtained as a necessary condition for equalizing the two expressions of the elastic constant C_{44} obtained by solving Eq. (1) in the long-wavelength limit approached from the two symmetry directions [0001] and [01$\bar{1}$0]. In Eq. (8) we have used the symbol α_j for A_j/r_j.

Equation (1) breaks into second-order determinantal equations in the symmetry directions [0001] and [01$\bar{1}$0] and can be easily solved to obtain expressions for the vibration frequencies in analytical forms. These expressions take still simpler forms for the zone-center and the zone-boundary points along the two principal symmetry directions. The expressions for the elastic constants are obtained by equating the 3×3 acoustic-mode dynamical matrix to the elastic matrix of the solid exactly as described by de Wames *et al.*[3] The expressions for the elastic constants thus obtained are given below, together with the expressions for some of the vibration frequencies corresponding to the zone-center and zone-boundary points in the symmetry directions. The subscripts LO and TO with the frequencies for the zone center Γ indicate, respectively, the longitudinal and transverse frequencies of the [0001] direction:

$$C_{11} = \frac{\sqrt{3}}{2c}\left(\frac{4}{3}\,(3\alpha_1 + \alpha_2 + 4\alpha_3 + 14\,\alpha_5) + 3\beta_1 + \beta_2 + 4\beta_3 + 14\,\beta_5 - \frac{(\beta_2 - 2\beta_3 + \frac{20}{7}\,\beta_5)^2}{6(\alpha_2 + \alpha_3 + 2\alpha_5) + 3(\beta_2 + \beta_3 + 2\beta_5)}\right) + K_e \quad , \tag{9}$$

$$C_{12} = \frac{\sqrt{3}}{2c}\left(-\frac{4}{3}\,(3\alpha_1 + \alpha_2 + 4\alpha_3 + 14\,\alpha_5) + \frac{1}{3}\,(3\beta_1 + \beta_2 + 4\beta_3 + 14\beta_5) + \frac{(\beta_2 - 2\beta_3 + \frac{20}{7}\,\beta_5)^2}{6(\alpha_2 + \alpha_3 + 2\alpha_5) + 3(\beta_2 + \beta_3 + 2\beta_5)}\right) + K_e \quad , \tag{11}$$

$$C_{33} = (\sqrt{3}\,c/6a^2)\,[6(\alpha_2 + \alpha_3 + 2\alpha_5) + \tfrac{9}{2}\,(c^2/a^2)\,(\beta_2 + \tfrac{1}{4}\,\beta_3 + \tfrac{2}{7}\,\beta_5) + 8(\alpha_4 + \beta_4)] + K_e \quad ,$$

$$C_{44} = (\sqrt{3}\,c/a^2)\,(\alpha_2 + \alpha_3 + 2\alpha_5 + \tfrac{4}{3}\,\alpha_4) + (\sqrt{3}c/2a^2)\,(\beta_2 + 2\beta_3 + 2\beta_5) \quad , \tag{12}$$

$$C_{13} + C_{44} = (\sqrt{3}c/a^2)\,(\beta_2 + \beta_3 + 2\beta_5) + K_e \quad , \tag{13}$$

$$m\omega^2_{\mathrm{LO}}(\Gamma) = 2[6(\alpha_2 + \alpha_3 + 2\alpha_5) + \tfrac{9}{2}\,(c^2/a^2)\,(\beta_2 + \tfrac{1}{4}\,\beta_3 + \tfrac{2}{7}\,\beta_5)] \quad , \tag{14}$$

$$m\omega^2_{\mathrm{TO}}(\Gamma) = 6[2(\alpha_2 + \alpha_3 + 2\alpha_5) + \beta_2 + \beta_3 + 2\beta_5] \quad , \tag{15}$$

$$m\omega^2_{\mathrm{LA}}(A) = 6(\alpha_2 + \alpha_3 + 2\alpha_5) + \tfrac{9}{2}\,(c^2/a^2)\,(\beta_2 + \tfrac{1}{4}\,\beta_3 + \tfrac{2}{7}\,\beta_5) + 4(\alpha_4 + \beta_4) + K_e G^2 k_m^2\,\Omega \quad , \tag{16}$$

$$m\omega^2_{\mathrm{TA}_\perp}(M) = 4(2\alpha_1 + \alpha_2 + 3\alpha_3 + 2\alpha_5) + 3(c^2/a^2)\,(\beta_2 + \tfrac{3}{4}\,\beta_3 + \tfrac{2}{7}\,\beta_5) \quad , \tag{17}$$

$$m\omega^2_{\mathrm{TO}_\perp}(M) = 8(\alpha_1 + \alpha_2 + 2\alpha_5) + 6(c^2/\alpha^2)(\beta_2 + \tfrac{2}{7}\beta_4) , \tag{18}$$

where k_m is the maximum value of k in the [0001] direction. For convenience we have used the substitutions

$$\beta_1 = B_1 - \frac{A_1}{r_1} \;, \quad \beta_2 = \frac{B_2 - A_2/r_2}{1 + 3c^2/4a^2} \;, \quad \beta_3 = \frac{B_3 - A_3/r_3}{1 + 3c^2/16a^2} \;, \quad \beta_4 = B_4 - \frac{A_4}{r_4} \;, \quad \beta_5 = \frac{B_5 - A_5/r_5}{1 + 3c^2/28a^2} \quad .$$

These equations form a complete set for the determination of the eleven parameters α_j, β_j ($j = 1$, 2, 3, 4, 5), and K_e of the theory. These parameters can be substituted into Eqs. (4) and (5) to obtain the coupling coefficients for many different values of k along the symmetry directions [0001] and [01$\bar{1}$0]. Solution of Eq. (1) leads to the frequencies ω which can be plotted against wave number k to give the dispersion curves.

III. RESULTS AND DISCUSSIONS

The theory described in Sec. II has been used to derive the dispersion curves of a number of hexagonal metals. We are reporting here the results

TABLE I. Input data: elastic constants in units of 10^{12} dyn cm^{-2} and vibration frequencies in 10^{12} sec^{-1}.

Property	Magnesium	Scandium	Zirconium	Holmium
a(Å)	3.2094	3.3090	3.2331	3.5773
c(Å)	5.2105	5.2680	5.1491	5.6158
m(amu)	24.312	44.956	91.23	164.93
C_{11}	0.5943[a]	0.993[b]	1.435[c]	0.7611[d]
C_{12}	0.2560[a]	0.457[b]	0.725[c]	0.2484[d]
C_{33}	0.6164[a]	1.069[b]	1.649[c]	0.7764[d]
C_{44}	0.1642[a]	0.277[b]	0.3207[c]	0.2571[d]
C_{13}	0.2140[a]	0.294[b]	0.654[c]	0.2060[d]
$\nu_{LO}(\Gamma)$	7.3[e]	6.91[f]	4.596[g]	3.4[h]
$\nu_{TO}(\Gamma)$	3.75[e]	4.04[f]	2.611[g]	1.94[h]
$\nu_{LA}(A)$	5.2[e]	4.74[f]	5.643[g]	2.56[h]
$\nu_{TA}(M)$	4.15[e]	3.97[f]	2.698[g]	1.96[h]
$\nu_{TO}(M)$	6.12[e]	6.23[f]	4.812[g]	3.04[h]

[a] Slutsky and Garland, Ref. 16.

[b] Fisher and Dever, Ref. 17.

[c] Fisher and Ranken, Ref. 18.

[d] Lahteenkorva, Ref. 10.

[e] Iyengar *et al.*, Ref. 2.

[f] Wakabayashi *et al.*, Ref. 13.

[g] Bezdek *et al.*, Ref. 14.

[h] Nicklow *et al.*, Ref. 5.

TABLE II. Atomic force constants in units of 10^4 dyn cm^{-1} and bulk modulus K_e in 10^{12} dyn cm^{-2}.

Parameter	Magnesium	Scandium	Zirconium	Holmium
α_1	0.013 86	0.125 75	0.347 73	0.102 87
α_2	0.015 92	0.131 98	0.318 40	0.186 87
α_3	−0.035 15	−0.126 62	−0.387 02	−0.061 36
α_4	0.000 50	−0.051 32	0.027 16	−0.000 61
α_5	0.001 59	−0.037 92	0.009 89	0.031 93
β_1	0.998 77	1.862 00	1.080 19	1.080 19
β_2	0.356 82	0.607 01	0.499 66	0.499 66
β_3	0.021 32	−0.010 20	−0.093 31	−0.093 31
β_4	−0.023 18	0.327 04	−0.246 79	−0.246 79
β_5	0.013 70	0.172 90	−0.053 45	−0.053 45
K_e	0.022 88	−0.214 55	0.311 52	0.235 52

for Mg, Sc, Zr, and Ho. The input data and the corresponding values of the parameters are given in Tables I and II. Phonon frequencies were calculated for a number of wave vectors in the symmetry directions [0001] and [01$\bar{1}$0]. These frequencies were then plotted against wave number k to obtain the dispersion curves for the elements Mg, Sc, Zr, and Ho, which are shown, respectively, in Fig. 1–4 by solid lines. The theoretical curves so obtained have been compared with the experimental points of Iyengar *et al.*,[2] Wakabayashi *et al.*,[13] Nicklow *et al.*,[5] and Bezdek *et al.*[14] The input data and hence the calculated dispersion curves correspond to room temperature. The dashed curves shown in the figures have been determined by the use of seven-neighbor central-force-constant model[15] with the electron ion-interaction used in the present study. The calculations based on five-neighbor central pair potentials show a significant improvement over the seven-neighbor calculations and generally present a very good agreement with the corresponding experimental data. In particular, along the [0001] symmetry direction there is almost an exact coincidence between theoretical and experimental curves. Some deviations are, however, seen in the [01$\bar{1}$0] direction which are largest near the zone boundary. While in the case of Mg and Sc these deviations are

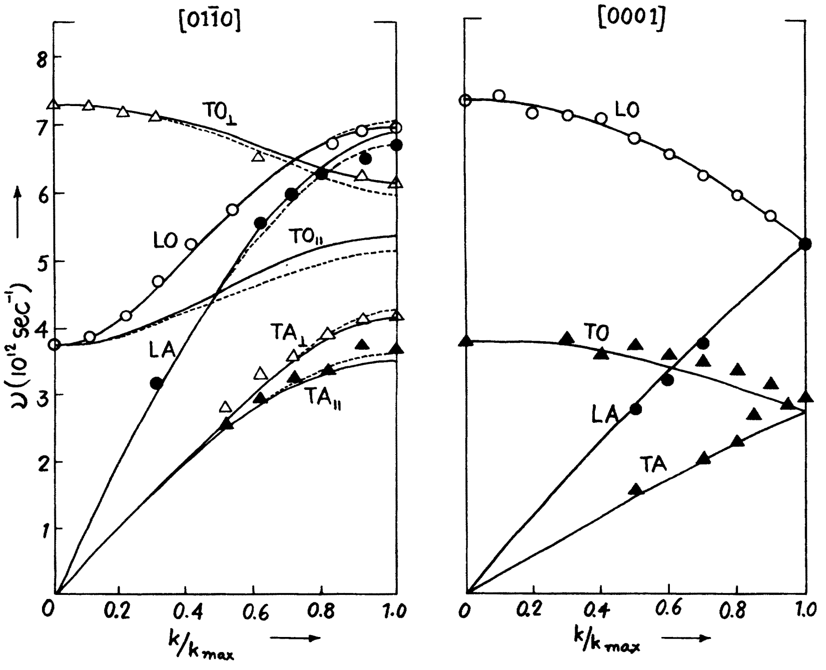

FIG. 1. Dispersion curves of Mg: solid curves according to five-neighbor central-pair-potential calculation; dashed curves according to seven-neighbor central-force-constant model; △, ▲, ○, ●, experimental points of Iyengar *et al.* (Ref. 2).

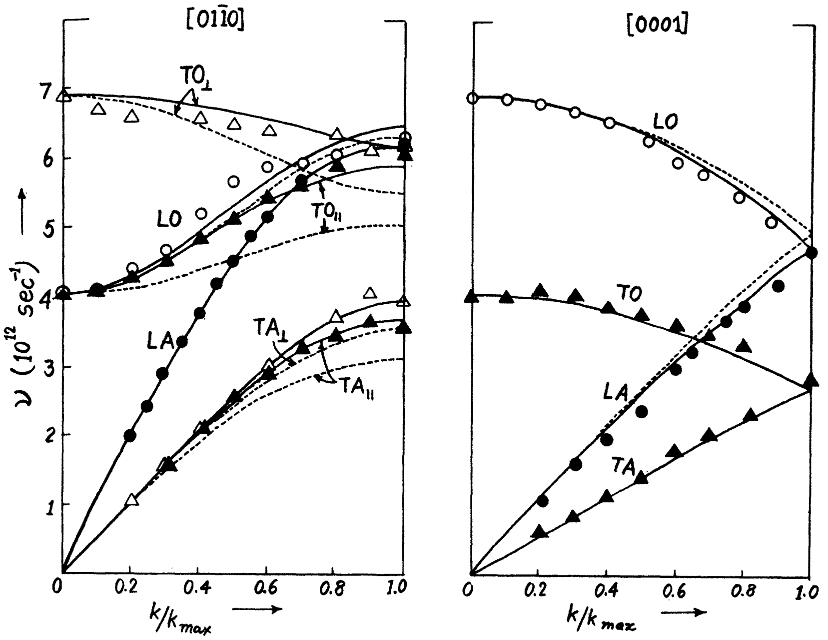

FIG. 2. Dispersion curves of Sc: solid curves according to five-neighbor central-pair-potential calculation; dashed curves according to seven-neighbor central-force-constant model; △,▲,○,●, experimental points of Wakabayashi *et al.* (Ref. 13).

insignificant, they increase to 7% for Zr and 10% for Ho. A least-squares-fitting program can be used to reduce the differences between the theoretical and experimental curves, leading perhaps to exact agreement. The order of agreement obtained by us generally compares very well with those obtained by other workers. Therefore, our model with only ten independent parameters, as against 13 or more used in other current models, should receive attention of theoretical workers studying lattice dynamics of hcp metals.

A look at Eqs. (12) and (15) shows that C_{44} and $\omega_{\mathrm{TO}}^{(\Gamma)}$ contain identical combinations of the force constants α_j and β_j but for a term in α_4 which appears in C_{44} and not in $\omega_{\mathrm{TO}}(\Gamma)$. It appears, therefore, that in absence of a fourth-neighbor ion-ion inter-

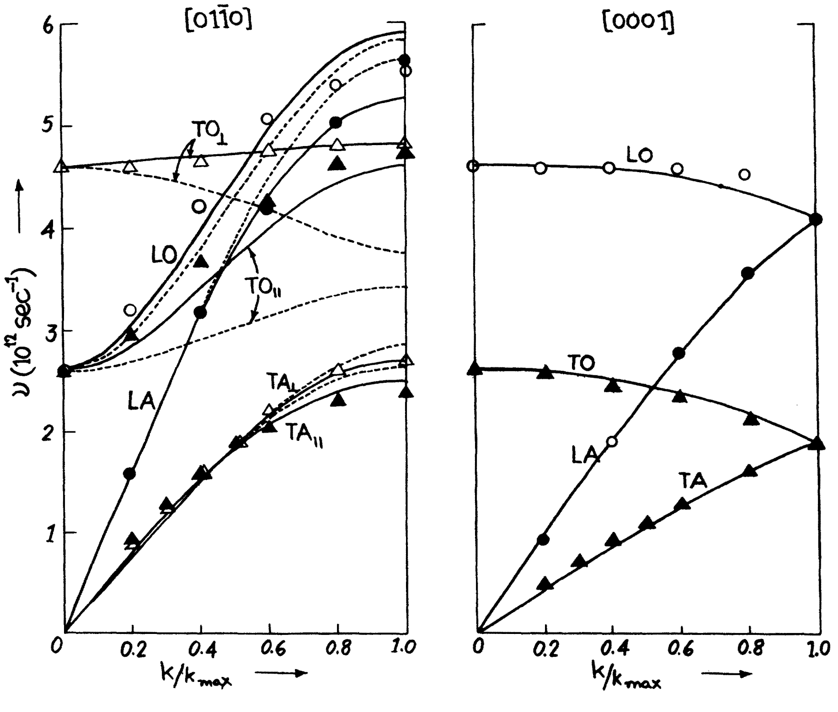

FIG. 3. Dispersion curves of Zr: solid curves according to five-neighbor central-pair-potential calculation; dashed curves according to seven-neighbor central-force-constant model; △,▲,○,●, experimental points of Bezdek *et al.* (Ref. 14).

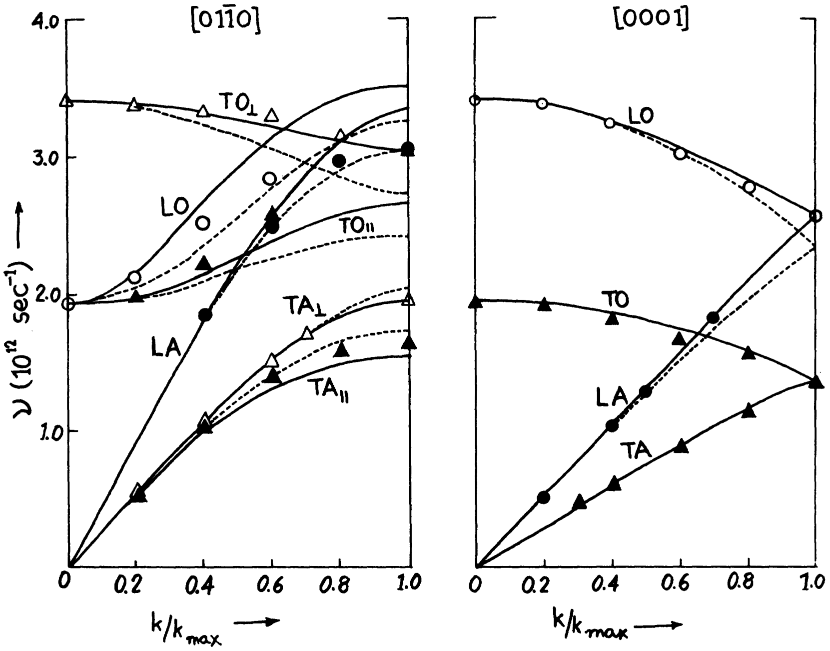

FIG. 4. Dispersion curves of Ho: solid curves according to five-neighbor central-pair-potential calculation; dashed curves according to seven-neighbor central-force-constant model; △,▲,○,●, experimental points of Nicklow *et al.* (Ref. 5).

action, C_{44} and $\omega_{TO}(\Gamma)$ could be related through an identity containing the lattice parameters and density of the solid. Such an identity is not satisfied by the values of C_{44} and $\omega_{TO}(\Gamma)$ of the hcp metals in general. Obviously, inclusion of fourth-neighbor ion-ion interaction is important in the present scheme and the same is true of the tensor-force models. It appears that the ion-ion interaction in hcp metals must extend at least up to the fourth neighbors. In case this interaction is represented by central forces implying first derivatives α_j of the potentials ϕ_j^i equal to zero, the identity in C_{44} and $\omega_{TO}(\Gamma)$ is restored and can be broken only if the ion-ion interactions are extended to seventh neighbors. This suggests that the central pair potentials give a better representation of ion-ion interactions than the central forces in conventional for force-constant models.

The main reason for the small differences between theory and experiment seen in the figures seems to be the inexactness in the electron-ion interaction term. We may expect that a better electron-ion-interaction formulation, for example the use of a suitable model pseudopotential, with the five-neighbor central pair potential will present a good description of the dynamics of hcp lattices in general.

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[1] M. F. Collins, Proc. Phys. Soc. Lond. **80**, 362 (1962).

[2] P. K. Iyengar, G. Venkataraman, P. R. Vijayaraghavan, and A. P. Roy, in *Inelastic Scattering of Neutrons in Solids and Liquids* (International Atomic Energy Agency, Vienna 1965), Vol. 1, p. 153.

[3] R. E. de Wames, T. Wolfram, and G. W. Lehman, Phys. Rev. **138**, A717 (1965).

[4] J. C. G. Houmann and R. M. Nicklow, Phys. Rev. B **1**, 3943 (1970).

[5] R. M. Nicklow, N. Wakabayashi, and P. R. Vijayaraghavan, Phys. Rev. B **3**, 1229 (1971).

[6] Walter F. King and P. H. Cutler, Phys. Rev. B **3**, 2485 (1971).

[7] R. S. Leigh, B. Szigeti and V. K. Tewary, Proc. R. Soc. Lond. A **320**, 505 (1971).

[8] B. Szigeti, *Proceedings of the International Conference on Phonons, Rennes, France* (Flammarion, Paris, France, 1971).

[9] P. K. Sharma and S. K. Joshi, J. Chem. Phys. **39**, 2633 (1963).

[10] E. E. Lahteenkorva, Solid State Commun. **8**, 947 (1970).

[11] B. Sharan and R. P. Bajpai, J. Phys. Soc. Jap. **28**, 338 (1970).

[12] M. P. Verma and J. C. Upadhyaya, J. Phys. F **1**, 618 (1971).

[13] N. Wakabayshi, S. K. Sinha, and F. H. Spedding, Phys. Rev. B **4**, 2398 (1971).

[14] H. F. Bezdek, R. E. Schmunk, and L. Finegold, Phys. Status Solidi **42**, 275 (1970).

[15] J. C. Upadhyaya and M. P. Verma, J. Phys. F (to be published).

[16] L. J. Slutsky and C. W. Garland, Phys. Rev. **107**, 972 (1957).

[17] E. S. Fisher and D. Dever, in Proceedings of the Seventh Rare Earth Research Conference, Vol. 1, 237, 1968 (unpublished).

[18] E. S. Fisher and C. J. Renken, J. Nucl. Mater. **4**, 311 (1961).