Two relations between elastic constants and optical phonon frequencies in hcp crystals with not too extended interatomic interactions

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We note that if the interatomic interactions of the 11th or more distant neighbors in an hcp crystal are negligible, there exist two simple relations between the elastic constants C_{33} and C_{44} and the phonon frequencies at points A and Γ. Comparison of these relations to the experimental data can provide a direct information about the scale of the long-range interaction effects in hcp metals.

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I. INTRODUCTION

Features of interatomic interactions in metals related to the electron-ion and electron-electron correlations attract much attention (see, e.g., Refs. 1–4). It is usually believed that the correlation effects should enlarge the effective interaction range, and the manifestations of these effects in phonon spectra of transition metals were discussed by some authors.[1,2] However, it seems difficult to obtain any quantitative estimates for the effects considered within the phenomenological approaches used by these authors. Let us also note that the most probable origin for possible long-range interactions in metals seem to be just the correlation effects, as the electrostatic screening length is here usually quite short, while Friedel's tails in inter-ionic interactions are typically small and insignificant (see, e.g., Ref. 5).

In this Brief Report, we note that there exist two simple but nontrivial relations between the elastic constants and the phonon frequencies in an hcp crystal which are violated by interactions of only the 11th or more distant neighbors in the crystal. Thus, an experimental check of these relations can provide the quantitative information about the long-range interaction effects in hcp crystals, in particular, in many metals. For brevity, these relations will be called "the elastic-optic vibrational relations" (EOVRs).

The derivation of EOVR in this work is based on the analysis of the general form of the dynamical matrix of an hcp crystal illustrated by the seven-neighbor interaction model which is published elsewhere.[6] In Sec. II, we describe the necessary results of that analysis and extend it to the case of more distant interactions under consideration. In Sec. III, we derive the EOVR. In Sec. IV, we compare the predictions of EOVR to the available experimental data and discuss the results of this comparison.

II. DYNAMICAL MATRIX OF AN HCP CRYSTAL WITH INTERACTIONS IN THREE NEAREST BASAL PLANES

Let us denote the period of the hcp lattice along the hexagonal axis z as $\mathbf{c}$ and the periods in the basal plane (x,y) as $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3=-(\mathbf{b}_1+\mathbf{b}_2)$, where $|\mathbf{b}_s|$ is a. The components of the lattice vector $\mathbf{R}$ along and normal to the z axis are denoted as $\mathbf{H}$ and $\mathbf{r}$: $\mathbf{R}=\mathbf{H}+\mathbf{r}$. Atoms in basal planes with $\mathbf{H}=n\mathbf{c}$ and $\mathbf{H}=n\mathbf{c}+\mathbf{h}$ (where $\mathbf{h}=\mathbf{c}/2$) form sublattices 1 and 2 shifted relative to each other by the vector $\mathbf{R}_{21}=\mathbf{h}+\mathbf{d}_s$, where $\mathbf{d}_s$ is $(\mathbf{b}_{s+1}-\mathbf{b}_{s+2})/3$, and index s is 1, 2, or 3 being defined by modulo 3: $s+2=s-1$.

Let us write the pth vector in the nth atomic coordination sphere ("in the star n") as $\mathbf{R}_{np}=\mathbf{r}_{np}+\mathbf{H}_{np}$, and define the auxiliary unit vectors $\mathbf{n}_p$ and $\mathbf{n}_p^z$ by the relations

$$\mathbf{n}_p=\mathbf{r}_{np}/r_n, \quad \mathbf{n}_p^z=\mathbf{H}_{np}/H_n, \tag{1}$$

where $r_n=|\mathbf{r}_{np}|$ and $H_n=|\mathbf{H}_{np}|$. Then, in the standard representation of the force constant matrix $\mathbf{A}$ as the sum of matrices $A_n^{\alpha\beta}(\mathbf{R}_{np})=A_{np}^{\alpha\beta}$,[8] these matrices can be written in the following form convenient for general treatments[6]:

$$A_{np}^{\alpha\beta}=a_n n_p^\alpha n_p^\beta+b_n\delta_{\alpha\beta}^\perp+c_n\delta_{\alpha\beta}^{zz}+d_n(n_p^\alpha n_p^{z\beta}+n_p^{z\alpha}n_p^\beta)+e_n\varepsilon_{\alpha\beta}^\perp I_p. \tag{2}$$

Here, α and β are Cartesian indices; coefficients a_n, b_n, c_n, d_n, and e_n are the Born–von Karman (BvK) parameters; $\delta_{\alpha\beta}^\perp$ is the Kronecker symbol for transverse components; $\delta_{\alpha\beta}^{zz}$ is unity at $\alpha=\beta=z$ and zero otherwise; a_n is nonzero only when $r_n\neq 0$, while d_n is nonzero when both $r_n\neq 0$ and $H_n\neq 0$; and $\varepsilon_{\alpha\beta}^\perp=-\varepsilon_{\beta\alpha}^\perp$ is the unit antisymmetric tensor for transverse components. The last term in Eq. (2) with $I_p(\pm\mathbf{R}_{np})=\pm 1$ is nonzero only for some special stars n discussed in Ref. 6, but it makes no contribution to EOVR and will be not considered below.

To write the dynamical matrix, one should consider the differences of lattice vectors $\mathbf{R}_{np}^{kl}=(\mathbf{R}_k-\mathbf{R}_l)_{np}$, where indices k and l are equal to 1 or 2. To this end, it is convenient to denote the vectors $\mathbf{R}_{np}$ with $\mathbf{H}_{np}=\pm m\mathbf{h}$ belonging to the mth basal plane as $\mathbf{R}_{np}\{m\}$. Below, we mainly consider the interaction models with $m\leqslant 2$ which include interactions up to the 11th neighbor when the hexagonal ratio c/a exceeds 1.5811 (which is the case for the 15 of total 22 elemental hcp metals[7]) and up to the 10th neighbor at smaller c/a. Then, the differences $\mathbf{R}_{np}^{11}$ and $\mathbf{R}_{np}^{22}$ are $\mathbf{R}_{np}\{0\}$ or $\mathbf{R}_{np}\{2\}$, while the differences $\mathbf{R}_{np}^{12}=-\mathbf{R}_{np}^{21}$ are $\mathbf{R}_{np}\{1\}$. Vectors $\mathbf{R}_{np}\{m\}$ for the 11 nearest neighbors are

$$\{0\}: \mathbf{R}_0=0, \quad \mathbf{R}_{2p}=\pm\mathbf{b}_s, \quad \mathbf{R}_{4p}=\pm 2\mathbf{h},$$

$$\mathbf{R}_{6p}=\pm 3\mathbf{d}_s, \quad \mathbf{R}_{8p}=\pm 2\mathbf{b}_s,$$

$$\{1\}: \mathbf{R}_{1p}=-\mathbf{d}_s\pm\mathbf{h}, \quad \mathbf{R}_{3p}=2\mathbf{d}_s\pm\mathbf{h},$$

$$\mathbf{R}_{5p}=-\mathbf{d}_s\pm\mathbf{b}_{s\mp 1}\pm\mathbf{h}, \quad \mathbf{R}_{9p}=-\mathbf{d}_s\pm 2\mathbf{b}_s\pm\mathbf{h},$$

$$\mathbf{R}_{11p} = -\mathbf{d}_s \pm 2\mathbf{b}_{s\mp1} \pm \mathbf{h},$$

$$\{2\}: \mathbf{R}_{4p} = \pm 2\mathbf{h}, \quad \mathbf{R}_{7p} = \pm \mathbf{b}_s \pm 2\mathbf{h},$$

$$\mathbf{R}_{10p} = \pm 3\mathbf{d}_s \pm 2\mathbf{h}, \tag{3}$$

where $(-\mathbf{d}_s \pm \mathbf{b}_{s\mp1})$ means $(-\mathbf{d}_s + \mathbf{b}_{s-1})$ or $(-\mathbf{d}_s - \mathbf{b}_{s+1})$, and similarly applies for $(-\mathbf{d}_s \pm 2\mathbf{b}_{s\mp1})$.

The six-row dynamical matrix $\mathbf{D}(k)$ can be written in the form of three-row blocks $\mathbf{D}_{kl}(\mathbf{k})$ as follows[6]:

$$\begin{pmatrix} \mathbf{D}_{11} & \mathbf{D}_{12} \\ \mathbf{D}_{12}^* & \mathbf{D}_{11}^* \end{pmatrix} = \begin{pmatrix} \mathbf{A}_{\mathbf{k}}^{\{0\}} + \mathbf{A}_{\mathbf{k}}^{\{2\}} & \mathbf{A}_{\mathbf{k}}^{\{1\}} \\ \mathbf{A}_{\mathbf{k}}^{\{1\}*} & \mathbf{A}_{\mathbf{k}}^{\{0\}*} + \mathbf{A}_{\mathbf{k}}^{\{2\}*} \end{pmatrix}, \tag{4}$$

where three-row matrices $\mathbf{A}_{\mathbf{k}}^{\{m\}}$ are defined by the relations

$$A_{\mathbf{k},\alpha\beta}^{\{m\}} = \sum_{n\in\{m\}} A_{n\mathbf{k}}^{\alpha\beta}\{m\}, \quad A_{n\mathbf{k}}^{\alpha\beta}\{m\} = \sum_p A_{np}^{\alpha\beta} e^{-i\mathbf{k}R_{np}\{m\}} \tag{5}$$

and symbol $n \in \{m\}$ means that the star n belongs to the mth basal plane. If we sum the second equation in Eq. (5) over components $\mathbf{H}_{np}$, we can write matrices $\mathbf{A}_{n\mathbf{k}}\{m\}$ in the form of blocks of transverse and z components:

$$\mathbf{A}_{n\mathbf{k}}\{0\} = \begin{pmatrix} \mathbf{A}_n^{\perp} & 0 \\ 0 & c_n\sigma_n \end{pmatrix},$$

$$\mathbf{A}_{n\mathbf{k}}\{1\} = \begin{pmatrix} \mathbf{A}_n^{\perp}\cos(\mathbf{kh}) & -i\mathbf{A}_n^{\perp z}\sin(\mathbf{kh}) \\ -i\mathbf{A}_n^{z\perp}\sin(\mathbf{kh}) & c_n\sigma_n\cos(\mathbf{kh}) \end{pmatrix},$$

$$\mathbf{A}_{n\mathbf{k}}\{2\} = \begin{pmatrix} \mathbf{A}_n^{\perp}\cos(2\mathbf{kh}) & -i\mathbf{A}_n^{\perp z}\sin(2\mathbf{kh}) \\ -i\mathbf{A}_n^{z\perp}\sin(2\mathbf{kh}) & c_n\sigma_n\cos(2\mathbf{kh}) \end{pmatrix}, \tag{6}$$

where two-row matrices $\mathbf{A}_n^{\perp}$ and vectors $\mathbf{A}_n^{\perp z} = \mathbf{A}_n^{z\perp}$ are expressed via $e_{np} = \exp(-i\mathbf{kr}_{np})$ and $\sigma = \Sigma_p e_{np}$ as follows:

$$(A_n^{\perp})_{\alpha\beta} = b_n\delta_{\alpha\beta}^{\perp}\sigma_n + \sum_p (a_n n_p^{\alpha} n_p^{\beta} + e_n \varepsilon_{\alpha\beta}^{\perp} I_p) e_{np},$$

$$(A_n^{\perp z})_{\alpha} = d_n \sum_p n_p^{\alpha} e_{np}. \tag{7}$$

Points Γ and A in the Brillouin zone correspond to the wave vectors $\mathbf{k}_{\Gamma} = 0$ and $\mathbf{k}_A = \pi\mathbf{h}/2h^2$. If we denote the elements of the dynamical matrix (4) at these points as $D_{\alpha\beta}^{kl,\Gamma}$ and $D_{\alpha\beta}^{kl,A}$, and the elements $A_{0,,xx}^{\{m\}}$ or $A_{0,zz}^{\{m\}}$ in Eqs. (5) as $A_{\perp}^{\{m\}}$ or $A_{\parallel}^{\{m\}}$, then the nonzero elements $D_{\alpha\beta}^{11,\Gamma}$, $D_{\alpha\beta}^{12,\Gamma}$, and $D_{\alpha\beta}^{11,A}$ can be written as

$$D_{xx}^{11,\Gamma} = D_{yy}^{11,\Gamma} = A_{\perp}^{\{0\}} + A_{\perp}^{\{2\}}, \quad D_{zz}^{11,\Gamma} = A_{\parallel}^{\{0\}} + A_{\parallel}^{\{2\}},$$

$$D_{xx}^{11,A} = D_{yy}^{11,A} = A_{\perp}^{\{0\}} - A_{\perp}^{\{2\}}, \quad D_{zz}^{11,A} = A_{\parallel}^{\{0\}} - A_{\parallel}^{\{2\}},$$

$$D_{xx}^{12,\Gamma} = D_{yy}^{12,\Gamma} = A_{\perp}^{\{1\}}, \quad D_{zz}^{12,\Gamma} = A_{\parallel}^{\{1\}}, \tag{8}$$

while quantities $A_{\perp}^{\{m\}}$ and $A_{\parallel}^{\{m\}}$ are related to the BvK parameters a_n, b_n, and c_n as follows:

$$A_{\perp}^{\{m\}} = \sum_{n\in\{m\}} z_n\left(\frac{a_n}{2} + b_n\right), \quad A_{\parallel}^{\{m\}} = \sum_{n\in\{m\}} z_n c_n, \tag{9}$$

where z_n is the coordination number for the star n. In the derivation of Eq. (9), we took into account that each star n with $r_n \neq 0$ consists of triads of vectors $\mathbf{R}_s$ related to each other by turns around the z axis at $\pm 120°$, and the sums of $\mathbf{n}_s$ in Eq. (7) for these triads obey the relations

$$\sum_s \mathbf{n}_s = 0, \quad \sum_s n_s^{\alpha} n_s^{\beta} = 3\delta_{\alpha\beta}^{\perp}/2. \tag{10}$$

Note also that the translation invariance conditions, $\Sigma_l D_{\alpha\beta}^{kl,\Gamma} = 0$,[8] imply the quantities $A_{\perp}^{\{m\}}$ and $A_{\parallel}^{\{m\}}$ in Eq. (8) to obey the relations

$$\sum_{m=0}^{2} A_{\perp}^{\{m\}} = 0, \quad \sum_{m=0}^{2} A_{\parallel}^{\{m\}} = 0. \tag{11}$$

Eigenvalues λ_i of the dynamical matrix are related to the phonon frequencies ω_i as $\lambda_i = M\omega_i^2$, where M is atomic mass. Using Eqs. (4), (8), and (11), we can express the sums $A_{\perp}^{\{m\}}$ and $A_{\parallel}^{\{m\}}$ in Eqs. (9) via the phonon frequencies ω_i at points Γ and A:

$$A_{\perp}^{\{1\}} = -M\omega_{\perp}^2(\Gamma_5^+)/2, \quad A_{\parallel}^{\{1\}} = -M\omega_{\parallel}^2(\Gamma_3^+)/2,$$

$$A_{\perp}^{\{0,2\}} = M[\omega_{\perp}^2(\Gamma_5^+)/4 \pm \omega_{\perp}^2(A_3)/2],$$

$$A_{\parallel}^{\{0,2\}} = M[\omega_{\parallel}^2(\Gamma_3^+)/4 \pm \omega_{\parallel}^2(A_1)/2], \tag{12}$$

where we use the standard notation for phonon modes (see, e.g., Ref. 9), while symbols $\perp$ or $\parallel$ mean the phonon polarization to be normal or parallel to the z axis.

III. RELATIONS BETWEEN THE ELASTIC CONSTANTS C_{33} AND C_{44} AND THE PHONON FREQUENCIES AT POINTS A AND Γ

Expressions for the elastic moduli $c_{\alpha\gamma,\beta\delta}$ via the BvK parameters can be found from the expansion of the dynamical matrix $\mathbf{D}(\mathbf{k})$ at small k.[8] As an hcp crystal has no inversion symmetry, these expressions include two different terms: $c_h^{\alpha\gamma,\beta\delta}$ related to the homogeneous shift of all atoms of an elementary cell in the long-wave acoustic mode under consideration, and $c_r^{\alpha\gamma,\beta\delta}$ related to the relative atomic displacements in this mode:

$$c_{\alpha\gamma,\beta\delta} = c_h^{\alpha\gamma,\beta\delta} + c_r^{\alpha\gamma,\beta\delta}. \tag{13}$$

To find tensors $\mathbf{c}_h$ and $\mathbf{c}_r$, we expand matrices $\mathbf{D}_{kl}(\mathbf{k})$ in Eq. (4) at small k,

$$D_{11}^{\alpha\beta}(\mathbf{k})|_{k\to0} = \sum_{\gamma\delta} d_{11}^{\alpha\beta,\gamma\delta} k_{\gamma} k_{\delta},$$

$$D_{12}^{\alpha\beta}(\mathbf{k})|_{k\to0} = -i\sum_{\gamma} d_{12}^{\alpha\beta\gamma} k_{\gamma} + \sum_{\gamma\delta} d_{12}^{\alpha\beta,\gamma\delta} k_{\gamma} k_{\delta}, \tag{14}$$

and define the tensor $\mathbf{d}$ by the relation

TABLE I. Comparison of experimental elastic constants C_{44} and C_{33} (in GPa) to those calculated using Eqs. (22).

Metal	Be	Mg	Zn	Cd	Tl	Sc	Ti	Co	Y	Zr	Tc	Ru	Hf	Re	Tb	Ho	Lu
c/a	1.58	1.62	1.86	1.89	1.60	1.59	1.59	1.62	1.57	1.59	1.6 1	1.56	1.58	1.62	1.58	1.57	1.59
C_{44}^{expt}	163	16.4	39.6	19	7.2	27.7	46.5	71	24.5	33.4	177	181	55.7	161	21.6	25.9	26.8
C_{44}^{EOVR}	137	24	35	18	7	34	44	63	29.6	28	98	152	60	136	22.2	23.4	33.6
ΔC_{44}^{EOVR}	±30	±1	±1	±3	±5	±1	±4	±6	±1.5	±1.5	±10	±15	±15	±15	±1.5	±1	±1
C_{33}^{expt}	349	61.5	61.8	49.9	36	107	181	335	78	166	470	624	197	683	73.3	7 9.6	80.9
C_{33}^{EOVR}	350	64	54	47	30	86	240	430	70	203	730	550	220	910	85	100	75
ΔC_{33}^{EOVR}	±55	±5	±2	±6	±15	±2	±15	±35	±4	±10	±30	±40	±30	±40	±5	±4	±2
Source of data on ω_i	Ref. 11	Ref. 12	Ref. 13	Ref. 14	Ref. 15	Ref. 16	Ref. 2	Ref. 2	Ref. 17	Ref. 18	Ref. 2	Ref. 2	Ref. 19	Ref. 2	Ref. 9	Ref. 20	Ref. 21

$$d_{\alpha\beta,\gamma\delta} = d_{11}^{\alpha\beta,\gamma\delta} + d_{12}^{\alpha\beta,\gamma\delta}. \quad (15)$$

Then, the first term in Eq. (13) is expressed via the components $d_{\alpha\beta,\gamma\delta}$ in Eq. (15) as follows[8]:

$$c_h^{\alpha\gamma,\beta\delta} = (d_{\alpha\beta,\gamma\delta} + d_{\beta\gamma,\alpha\delta} - d_{\beta\delta,\alpha\gamma})/\Omega_a, \quad (16)$$

where Ω_a is volume per atom. The second term in Eq. (13) makes no contribution to the elastic constants C_{33} and C_{44} discussed in this Brief Report [it affects only constant $\tilde{B}$ in Eq. (21)]; thus, this term is not considered below.

Using Eqs. (4) and (5), we can express the tensor $\mathbf{d}$ in Eq. (15) via matrices $\mathbf{A}_{np}$ in Eq. (2) as follows:

$$d_{\alpha\beta,\gamma\delta} = \sum_n d_n^{\alpha\beta,\gamma\delta}, \quad d_n^{\alpha\beta,\gamma\delta} = -\sum_p R_{np}^{\gamma} R_{np}^{\delta} A_{np}^{\alpha\beta}/2. \quad (17)$$

Summations over vectors p in Eq. (17) can be easily made if we write $\mathbf{R}_{np}$ as $r_n\mathbf{n}_p + H_n\mathbf{n}_p^z$ and use both Eqs. (10) and similar relations for products of four-vectors $\mathbf{n}_s$:

$$\sum_s n_s^{\alpha} n_s^{\beta} n_s^{\gamma} n_s^{\delta} = 3\Delta_{\alpha\beta\gamma\delta}^{\perp}/8,$$

$$\Delta_{\alpha\beta\gamma\delta}^{\perp} = \delta_{\alpha\beta}^{\perp}\delta_{\gamma\delta}^{\perp} + \delta_{\alpha\gamma}^{\perp}\delta_{\beta\delta}^{\perp} + \delta_{\alpha\delta}^{\perp}\delta_{\beta\gamma}^{\perp}. \quad (18)$$

Therefore, each quantity $d_{\alpha\beta,\gamma\delta}/\Omega_a$ in Eq. (16) has the form

$$\begin{aligned} d_{\alpha\beta,\gamma\delta}/\Omega_a = {} & A\Delta_{\alpha\beta\gamma\delta}^{\perp} + B\delta_{\alpha\beta}^{\perp}\delta_{\gamma\delta}^{\perp} + C\delta_{\alpha\beta}^{\perp}\delta_{\gamma\delta}^{zz} + D\delta_{\alpha\beta}^{zz}\delta_{\gamma\delta}^{\perp} \\ & + E\delta_{\alpha\beta}^{zz}\delta_{\gamma\delta}^{zz} + F(\delta_{\alpha\gamma}^{\perp}\delta_{\beta\delta}^{zz} + \delta_{\beta\delta}^{\perp}\delta_{\alpha\gamma}^{zz} + \delta_{\alpha\delta}^{\perp}\delta_{\beta\gamma}^{zz} \\ & + \delta_{\beta\delta}^{\perp}\delta_{\alpha\gamma}^{zz}), \end{aligned} \quad (19)$$

where constants $A-F$ can be expressed via the BvK parameters using Eqs. (17), (2), (10), and (18). In particular, for the constants C and E, we obtain

$$C = -\frac{1}{4}\sum_n z_n(a_n + 2b_n)H_n^2, \quad E = -\frac{1}{2}\sum_n z_n c_n H_n^2. \quad (20)$$

Substituting Eq. (19) into Eq. (16), we find that the condition of symmetry of elastic moduli,[8] $c_{\alpha\gamma,\beta\delta} = c_{\beta\delta,\alpha\gamma}$, implies the relation $D=C$. Finally, we express the elastic constants C_{ik} (in standard Voigt notation[10]) via constants $A-F$ in Eq. (19) putting indices α, β, γ, and δ in our tensor equations equal to x, y, or z. It yields

$$C_{11} = 3A + \tilde{B}, \quad C_{12} = A - \tilde{B}, \quad C_{33} = E,$$

$$C_{13} = 2F - C, \quad C_{44} = C, \quad (21)$$

where constant $\tilde{B}$ differs from B in Eq. (19) due to the contribution of terms $c_r^{\alpha\gamma,\beta\delta}$ mentioned above.[6]

For the three-plane interaction models discussed in Sec. II, the sums over n in Eqs. (20) include contributions of only two planes $\{m\}$ with m equal to 1 and 2, and these contributions are proportional to quantities $A_{\perp}^{\{m\}}$ and $A_{\parallel}^{\{m\}}$ in Eqs. (9). Combining Eq. (9), (12), (20), and (21), we obtain the following relations between the elastic constants C_{44} and C_{33} and the phonon frequencies $\omega_i(A)$ and $\omega_i(\Gamma)$:

$$C_{44} = M[\omega_{\perp}^2(A_3) - \omega_{\perp}^2(\Gamma_5^+)/4]c/a^2\sqrt{3},$$

$$C_{33} = M[\omega_{\parallel}^2(A_1) - \omega_{\parallel}^2(\Gamma_3^+)/4]c/a^2\sqrt{3}, \quad (22)$$

where c and a are the hcp lattice parameters. The first and the second of these relations will be called "the transverse EOVR" and "the longitudinal EOVR."

IV. COMPARISON OF ELASTIC-OPTIC VIBRATIONAL RELATIONS TO THE EXPERIMENTAL DATA AND DISCUSSION

In Table I, we compare the predictions of EOVR [Eq. (22)] to the experimental data for 17 hcp metals. In this table, c/a is the hexagonal ratio taken from Ref. 7, C_{ii}^{expt} is the experimental elastic constant taken from Ref. 10, C_{ii}^{EOVR} is the right-hand side of Eq. (22) calculated with the experimental ω_i taken from the source quoted, and ΔC_{ii}^{expt} is the error in C_{ii}^{EOVR} estimated supposing the distribution of experimental errors in $\omega_i(A)$ and $\omega_i(\Gamma)$ to be noncorrelated and Gaussian. All the data in Table I usually correspond to room temperature.

The results presented in Table I can be analyzed from both experimental and theoretical points of view. Here, we present only two general comments.

(i) For the nontransition metals from Be to Tl, both the transverse and the longitudinal EOVR seem usually to hold within the scale of experimental errors. The disagreements for Zn and Mg (which formally exceed $\Delta C_{ii}^{\mathrm{EOVR}}$) can be related to underestimating the errors $\Delta\omega_i$ in the papers quoted. In particular, for Mg, the 30% disagreement in C_{44} is related to using for $\omega(A_3)$ in Eq. (22) the value 2.94 THz from Ref. 12, while using for it the value 2.72 THz implied by the BvK interpolation suggested in Ref. 22 yields $C_{44}^{\mathrm{EOVR}} \simeq 17$ GPa, in agreement with C_{44}^{expt}. Thus, more precise measurements of ω_i in Mg and Zn seem desirable.

(ii) For the transition and rare-earth metals, except for Tc, the transverse EOVR seems usually to hold within the scale of experimental errors, while the longitudinal EOVR typically overestimates C_{33} by about 20%. The violations of this tendency for Sc and Lu may deserve further experimental studies, similar to the case of Mg and Zn. For Hf, and possibly also for Y, Ru, and Tb, the deviations from EOVR can be insignificant. For Tc, both the transverse and the longitudinal EOVR are violated drastically.

Most of observations (ii) agree qualitatively with those made by Wakabayashi *et al.*[2] in their analysis of manifestations of the long-ranged interaction effects in phonon spectra of transition metals. These authors found such effects to be very strong in Tc and Re where they also lead to the drastic softening of the Γ_3^+ mode. These effects were also found to be quite pronounced for the longitudinal branch $[0,0,\zeta]$ in Ti, Zr, Co, and Hf, being somewhat less in Ru, while for the transverse branches such effects were not revealed, and in Sc and Y, Wakabayashi *et al.* did not observe any long-range interaction effects. All these conclusions are similar to those obtained in our analysis of data for the transition metals in Table I, with a possible exception for Hf. At the same time, the present approach also enables one to quantify the scale of the effects under consideration.

To conclude, presently the experimental examination of EOVR seems to provide mainly qualitative information about the scale of the long-range interaction effects in hcp metals. However, a further progress in accuracy of phonon measurements can allow making more definite and quantitative conclusions basing on such analyses.

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[1] P. B. Allen, Phys. Rev. B **16**, 5139 (1977).
[2] N. Wakabayashi, R. H. Scherm, and H. G. Smith, Phys. Rev. B **25**, 5122 (1982).
[3] S. Baroni, S. de Gironcoli, and A. Dal Corso, Rev. Mod. Phys. **73**, 515 (2001).
[4] S. Y. Savrasov and G. Kotliar, Phys. Rev. Lett. **90**, 056401 (2003).
[5] A. M. Bratkovsky, V. G. Vaks, and A. V. Trefilov, J. Phys. F: Met. Phys. **13**, 2517 (1983), Fig. 1.
[6] V. G. Vaks and K. Yu. Khromov (unpublished).
[7] C. Kittel, *Introduction to Solid State Physics*, 4th ed. (Wiley, New York, 1978), Table 1.4.
[8] M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Oxford University Press, Oxford, 1954).
[9] J. C. Glyden Houmann and R. M. Nicklow, Phys. Rev. B **1**, 3943 (1970).
[10] *Second and Higher Order Elastic Constants*, edited by A. Every and A. McCurdy, Landolt-Börnstein New Series, Group III, Vol. 29, Part A (Springer, Berlin, 1992), pp. 105–128.
[11] R. E. Schmunk, R. M. Brugger, P. D. Randolph, and K. A. Strong, Phys. Rev. **128**, 562 (1962).
[12] P. K. Iyengar, G. Venkataraman, P. R. Vijayaraghavan, and A. P. Roy, *Inelastic Scattering of Neutrons* (IAEA, Vienna, 1965), Vol. I, p. 153.
[13] L. Almquist and R. Stedman, J. Phys. F: Met. Phys. **1**, 785 (1971).
[14] B. Dorner, A. A. Chernyshov, V. V. Pushkarev, A. Yu. Rumyantsev, and R. Pynn, J. Phys. F: Met. Phys. **11**, 365 (1980).
[15] T. G. Worlton and R. E. Schmunk, Phys. Rev. B **3**, 4115 (1971).
[16] N. Wakabayashi, S. K. Sinha, and F. H. Spedding, Phys. Rev. B **4**, 2398 (1971).
[17] S. K. Sinha, T. O. Brun, L. D. Muhlstein, and J. Sakurai, Phys. Rev. B **1**, 2430 (1970).
[18] C. Stassis, J. Zarestky, D. Arch, O. D. McMasters, and B. N. Harmon, Phys. Rev. B **18**, 2632 (1978).
[19] C. Stassis, D. Arch, O. D. McMasters, and B. N. Harmon, Phys. Rev. B **24**, 730 (1982).
[20] R. M. Nicklow, N. Wakabayashi, and P. R. Vijayaraghavan, Phys. Rev. B **3**, 1229 (1971).
[21] J. Pleschiutschnig, O. Blaschko, and W. Reichardt, Phys. Rev. B **41**, 975 (1990).
[22] R. Pynn and G. L. Squires, Proc. R. Soc. London, Ser. A **326**, 347 (1972).