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Abstract

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CRYSTALLOGRAPHY

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ON THE THEORY OF QUASI-TRANSVERSE ELASTIC WAVES IN CRYSTALS

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In the present paper a method is set forth for the approximate determination of the velocity and displacement of a quasi-transverse elastic wave in an arbitrary crystal, based on comparison with a hexagonal crystal closest in elastic properties.

The fundamental equation for the propagation of elastic waves in crystals has the form

$$(\Lambda - \lambda)u = 0, \tag{1}$$

where $\Lambda = (\Lambda_{kl}) = (\lambda_{ikjl} n_i n_j)$; λ_{ikjl} is the tensor of elastic constants divided by the density of the medium; n_i are the components of the unit vector of the wave normal $\mathbf{n}$; $\lambda = v^2$ is the square of the phase velocity; u is the wave-displacement vector. The quantities λ_{ijkl} may, in a known manner, be replaced by the quantities c_{mn} $(m, n = 1, 2, 3, 4, 5, 6)$. For a hexagonal crystal (a transversely isotropic medium) the corresponding tensor Λ^0 may be represented in the following covariant form:

$$\Lambda^0 = a_0 + a_1 \mathbf{n} \cdot \mathbf{n} + a_2 \mathbf{e} \cdot \mathbf{e} + a_3 \mathbf{c} \cdot \mathbf{c}, \qquad \mathbf{c} = \frac{[\mathbf{en}]}{|[\mathbf{en}]|}, \tag{2}$$

where $\mathbf{e}$ is the unit vector of the symmetry axis, and the coefficients a_s, $s = 0, 1, 2, 3$, are expressed in terms of c_{mn} and $n_3 = \mathbf{e} \cdot \mathbf{n}$ as follows:

$$\begin{gathered} a_0 = \eta_1 + \eta_2 n_3^2, \qquad a_1 = \eta_3, \qquad a_2 = \eta_2 + \eta_4 n_3^2, \qquad a_3 = \eta_5(1 - n_3^2), \\ \eta_1 = c_{11} - c_{44} - c_{13}, \qquad \eta_2 = 2c_{44} + c_{13} - c_{11}, \qquad \eta_3 = c_{13} + c_{44}, \\ \eta_4 = c_{11} + c_{33} - 4c_{44} - 2c_{13}, \qquad \eta_5 = c_{44} + c_{66} + c_{13} - c_{11}. \end{gathered} \tag{3}$$

We shall determine the tensor Λ^0 from the condition*

$$F = ((\Lambda - \Lambda^0)^2)_c = \min, \tag{4}$$

where the vector **e** will be fixed in advance, on the basis of the symmetry of the crystal. From condition (4) it follows that the coefficients a_s satisfy the system of equations

$$\left((\Lambda-\Lambda^0)\frac{\partial\Lambda^0}{\partial a_s}\right)_c=0,$$

whence it follows that

$$\Lambda'_c=\mathbf{n}\Lambda'\mathbf{n}=\mathbf{e}\Lambda'\mathbf{e}=\mathbf{c}\Lambda'\mathbf{c}=0, \tag{5}$$

where $\Lambda'=\Lambda-\Lambda^0$. In this case $(\Lambda\Lambda^0)_c=(\Lambda^{02})_c$, $(\Lambda^0\Lambda')_c=0$, and

$$F=(\Lambda'^2)_c=(\Lambda\Lambda')_c=(\Lambda^2)_c-(\Lambda^{02})_c. \tag{6}$$

Expanding the system (5), we obtain

$$\begin{gathered}3a_0+a_1+a_2+a_3=\Lambda_c,\qquad a_0+a_3=\mathbf{c}\Lambda\mathbf{c},\\ a_0+a_1+a_2n_3^2=\mathbf{n}\Lambda\mathbf{n},\qquad a_0+a_1n_3^2+a_2=\mathbf{e}\Lambda\mathbf{e}.\end{gathered} \tag{7}$$

* The subscript c denotes the trace of a tensor.

The solutions of this system have the form

$$a_0=\frac{(1+n_3^2)[\mathbf{ec}]\,\Lambda\,[\mathbf{ec}]-\mathbf{n}\Lambda\mathbf{n}+n_3^2\mathbf{e}\Lambda\mathbf{e}}{2n_3^2},\quad a_1=\frac{\mathbf{n}\Lambda\mathbf{n}-n_3^2\mathbf{e}\Lambda\mathbf{e}-(1-n_3^2)[\mathbf{ec}]\,\Lambda\,[\mathbf{ec}]}{2n_3^2(1-n_3^2)},$$

$$a_2=\frac{(1-2n_3^2)\mathbf{n}\Lambda\mathbf{n}+n_3^2\mathbf{e}\Lambda\mathbf{e}-(1-n_3^2)[\mathbf{ec}]\,\Lambda\,[\mathbf{ec}]}{2n_3^2(1-n_3^2)}, \tag{8}$$

$$a_3=\frac{3n_3^2\mathbf{c}\Lambda\mathbf{c}-n_3^2\Lambda_c+\mathbf{n}\Lambda\mathbf{n}-[\mathbf{ec}]\,\Lambda\,[\mathbf{ec}]}{2n_3^2}.$$

For $n_3=0$, the solutions (8) for all a_3 reduce to the indeterminacy $\frac{0}{0}$. This is connected with the fact that in the system (7) the first equation becomes equal to the sum of the other three as a consequence of the relation $\Lambda_c=\mathbf{n}\Lambda\mathbf{n}+\mathbf{e}\Lambda\mathbf{e}+\mathbf{c}\Lambda\mathbf{c}$. Since for $\mathbf{e}\perp\mathbf{n}$, $\mathbf{c}\cdot\mathbf{c}=1-\mathbf{e}\cdot\mathbf{e}-\mathbf{n}\cdot\mathbf{n}$, expression (2) for Λ^0 takes the form

$$\Lambda^0=a_0+a_1\mathbf{n}\cdot\mathbf{n}+a_2\mathbf{e}\cdot\mathbf{e}. \tag{9}$$

A calculation analogous to (3)–(7) leads to the following values of a_s:

$$a_0 = \mathbf{c}\Lambda\mathbf{c}, \qquad a_1 = \mathbf{n}\Lambda\mathbf{n} - \mathbf{c}\Lambda\mathbf{c}, \qquad a_2 = \mathbf{e}\Lambda\mathbf{e} - \mathbf{c}\Lambda\mathbf{c}.$$

These expressions also follow from the system (7), if one sets there $n_3 = a_3 = 0$. Returning to the general relations (5), we note that, according to (1):

$$[\mathbf{en}] \cdot [\mathbf{en}] = [\mathbf{en}]^2 + \mathbf{e} \cdot \mathbf{n}\,(\mathbf{e} \cdot \mathbf{n} + \mathbf{n} \cdot \mathbf{e}) - (\mathbf{e} \cdot \mathbf{e} + \mathbf{n} \cdot \mathbf{n}), \tag{10}$$

therefore one more condition is added to the conditions (5):

$$\mathbf{e}\Lambda'\mathbf{n} = \mathbf{n}\Lambda'\mathbf{e} = 0. \tag{11}$$

From (5), (11) the relations follow

$$\mathbf{n} \perp \Lambda'\mathbf{n} \perp \mathbf{e}, \qquad \mathbf{e} \perp \Lambda'\mathbf{e} \perp \mathbf{n}, \qquad \Lambda'\mathbf{e} \parallel \Lambda'\mathbf{n} \parallel [\mathbf{en}] \parallel \mathbf{c}. \tag{12}$$

Introduce the notation

$$\Lambda'\mathbf{c} = \mathbf{w}, \qquad \mathbf{w} \cdot \mathbf{c} = 0. \tag{13}$$

According to (12), $\Lambda'\mathbf{e} = k_1\mathbf{c}$, $\Lambda'\mathbf{n} = k_2\mathbf{c}$; multiplying these equalities scalarly by $\mathbf{c}$, we find $k_1 = \mathbf{w} \cdot \mathbf{e}$, $k_2 = \mathbf{w} \cdot \mathbf{n}$. Thus, we know the result of the action of the matrix Λ' on three independent vectors $\mathbf{c}, \mathbf{e}, \mathbf{n}$. Hence we find for Λ' (see (2))

$$\Lambda' = \frac{\mathbf{w} \cdot [\mathbf{en}] + \mathbf{we} \cdot \mathbf{c} \cdot [\mathbf{nc}] + \mathbf{wn} \cdot \mathbf{c} \cdot [\mathbf{ce}]}{[\mathbf{en}]\,\mathbf{c}} = \mathbf{w} \cdot \mathbf{c} + \mathbf{c} \cdot \mathbf{w}. \tag{14}$$

As a result, for the tensor Λ in any crystal we obtain the following representation:

$$\Lambda = \Lambda^0 + \Lambda' = a_0 + a_1\mathbf{n} \cdot \mathbf{n} + a_2\mathbf{e} \cdot \mathbf{e} + a_3\mathbf{c} \cdot \mathbf{c} + \mathbf{w} \cdot \mathbf{c} + \mathbf{c} \cdot \mathbf{w}. \tag{15}$$

We note that from (14), (13) there follows the relation

$$\mathbf{w}^2 = \frac{1}{2}(\Lambda'^2)_c = \frac{1}{2}F. \tag{16}$$

For a transversely isotropic medium, the equation $\Lambda^0\mathbf{u}_0 = \lambda_0\mathbf{u}_0$ always has the solution $\mathbf{u}_0 = \mathbf{c}$, $\lambda_0 = a_0 + a_3$. In the general case we shall seek a solution in the form

$$\mathbf{u} = \mathbf{c} + \mathbf{u}', \qquad \mathbf{u}' \cdot \mathbf{c} = 0, \qquad \lambda = a_0 + a_3 + \lambda'. \tag{17}$$

From (15)–(17), after multiplication by $\mathbf{c}$, it follows that

$$\lambda' = \mathbf{w}\cdot\mathbf{u}'. \tag{18}$$

As a result, equation (16) takes the form

$$(a_3 - a_1\mathbf{n}\cdot\mathbf{n} - a_2\mathbf{e}\cdot\mathbf{e})\mathbf{u}' = \mathbf{w} - \mathbf{w}\mathbf{u}'\cdot\mathbf{u}'. \tag{19}$$

For $n_3 = 0$, in an analogous way we arrive at the equation

$$(a_1\mathbf{n}\cdot\mathbf{n} + a_2\mathbf{e}\cdot\mathbf{e})\mathbf{u}' = -\mathbf{w} + \mathbf{w}\mathbf{u}'\cdot\mathbf{u}'. \tag{20}$$

Introducing the matrix

$$\gamma = (a_3 - a_1\mathbf{n}\cdot\mathbf{n} - a_2\mathbf{e}\cdot\mathbf{e})^{-1} = \frac{a_3^2 + a_3(a_1\mathbf{n}^{*2} + a_2\mathbf{e}^{*2}) + a_1a_2[\mathbf{en}]\cdot[\mathbf{en}]}{a_3(a_3(a_3 - a_1 - a_2) + a_1a_2[\mathbf{en}]^2)}, \tag{21}$$

we obtain from (19)

$$\mathbf{u}' = \gamma\mathbf{w} - \mathbf{w}\mathbf{u}'\cdot\gamma\mathbf{u}'. \tag{22}$$

This nonlinear equation is of the same form as for the case of quasif longitudinal waves. If $|\gamma\mathbf{w}| \ll 1$, it admits an approximate solution by simple iteration. Putting

$$\mathbf{u}'_1 = \gamma\mathbf{w}, \qquad \lambda'_k = \mathbf{w}\cdot\mathbf{u}'_k, \tag{23}$$

we obtain successive approximations by means of the recurrence formula

$$\mathbf{u}'_{k+1} = \gamma\mathbf{w} - \mathbf{w}\mathbf{u}'_k\cdot\gamma\mathbf{u}'_k. \tag{24}$$

The case $\mathbf{n}\cdot\mathbf{e} = 0$ requires a somewhat different approach, since in equation (20) $|a_1\mathbf{n}\cdot\mathbf{n} + a_2\mathbf{e}\cdot\mathbf{e}| = 0$. However, if one takes into account that $\mathbf{n}\cdot\mathbf{c} = \mathbf{e}\cdot\mathbf{c} = \mathbf{w}\cdot\mathbf{c} = \mathbf{u}'\cdot\mathbf{c} = 0$, i.e., that all the vectors $\mathbf{n}, \mathbf{e}, \mathbf{w}, \mathbf{u}'$ lie in one plane, then equation (20) reduces to a two-dimensional one. Therefore the matrix standing on the left at $\mathbf{u}'$ admits inversion, and the inverse matrix has the form

$$\sigma = \frac{\mathbf{n}\cdot\mathbf{n}}{a_1} + \frac{\mathbf{e}\cdot\mathbf{e}}{a_2}. \tag{25}$$

As a result, equation (20) likewise takes a form analogous to (24):

$$\mathbf{u}' = -\sigma \cdot \mathbf{w} + \mathbf{w}\mathbf{u}' \cdot \sigma \mathbf{u}'. \tag{26}$$

The rate of convergence of the series of successive approximations (24) is determined by the smallness of the quantity $|\gamma \mathbf{w}|$, an estimate of which can be obtained from data on the elastic constants of particular crystals. With the aid of (21), (13) we obtain

$$\gamma \mathbf{w} = \frac{b\mathbf{w} + a_1 \mathbf{wn} \cdot \mathbf{n} + a_2 \mathbf{we} \cdot \mathbf{e}}{a_3 b + a_1 a_2 [\mathbf{en}]^2}, \qquad b = a_3 - a_1 - a_2. \tag{27}$$

It is easy to see that $\mathbf{c}\gamma\mathbf{w} = \mathbf{c} \cdot \mathbf{w} = 0$; consequently, $\gamma\mathbf{w}$, like $\mathbf{w}$, lies in the meridional plane $(\mathbf{e}, \mathbf{n})$. Let us introduce the notation

$$\Delta = a_3 b + a_1 a_2 (1 - n_3^2) = (a_3 - a_1)(a_3 - a_2) - a_1 a_2 n_3^2. \tag{28}$$

Using (21), (13), (10), it is not difficult to verify the validity of the relation

$$\gamma^2 \mathbf{w} = \frac{(b + a_3)\gamma\mathbf{w} - \mathbf{w}}{\Delta}. \tag{29}$$

Hence it is clear that, for any approximation, the equality

$$\mathbf{u}'_k = \xi_k \gamma \mathbf{w} + \zeta_k \mathbf{w}, \tag{30}$$

will hold, and from (24), (29) the following recurrence formulas for the coefficients ξ_k, η_k follow:

$$\begin{aligned} \xi_{k+1} &= 1 - \frac{b + a_3}{\Delta} \xi_k (\xi_k \mathbf{w}\gamma\mathbf{w} + \zeta_k \mathbf{w}^2), \\ \zeta_{k+1} &= (\xi_k \mathbf{w}\gamma\mathbf{w} + \zeta_k \mathbf{w}^2)(\xi_k - \xi_k/\Delta). \end{aligned} \tag{31}$$

For the zeroth approximation, $u'_0 = 0,\ \xi_0 = \zeta_0 = 0$; for the first approximation, according to (31), $\xi_1 = 1,\ \zeta_1 = 0$, in agreement with (23). In the second approximation

$$u'_2 = \gamma\mathbf{w} - \mathbf{w}\gamma\mathbf{w} \cdot \gamma^2 \mathbf{w} = \left(1 - \frac{b + a_3}{\Delta} \mathbf{w}\gamma\mathbf{w}\right) \gamma\mathbf{w} - \frac{\mathbf{w}\gamma\mathbf{w}}{\Delta} \mathbf{w}. \tag{32}$$

Here, according to (18), (27), the correction of the first approximation to the eigenvalue λ'_1 is equal to

$$\lambda'_1 = \mathbf{w}\gamma\mathbf{w} = \frac{1}{\Delta} \left(b w^2 + a_1 (\mathbf{wn})^2 + a_2 (\mathbf{we})^2 \right). \tag{33}$$

In the second approximation we obtain, respectively,

$$\lambda_2' = \mathbf{w} u_2' = \mathbf{w}\gamma\mathbf{w}\left(1 - \frac{w^2 + (b + a_3)\,\mathbf{w}\gamma\mathbf{w}}{\Delta}\right). \tag{34}$$

With the aid of (17), (18) we find for the displacement and velocity of the quasi-transverse wave in the k-th approximation $u_k = \mathbf{c} + u_k'$, $\lambda_k = v_k^2 = a_0 + a_3 + \mathbf{w} \cdot u_k'$, where u_k' is determined by formulas (30), (31). After this one can, without difficulty, find the remaining solutions of equation (1) in the same approximation.

Application of the proposed method to the case of tetragonal crystals shows that, even in the case of the strongest anisotropy, already the second approximation gives quite sufficient accuracy.

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CITED LITERATURE

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Note: Figure translations are in progress. See original paper for figures.

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