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F. I. Fedorov

1964

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Abstract

Full Text

Reports of the Academy of Sciences of the USSR

1964. Volume 155, No. 4

CRYSTALLOGRAPHY

F. I. FEDOROV

A GENERAL APPROXIMATE THEORY OF ELASTIC WAVES IN CRYSTALS

(Presented by Academician A. V. Shubnikov on 19 XII 1963)

As is known, the properties of plane elastic waves in homogeneous crystals are described by the equation

$$\Lambda \mathbf{u} = v^2 \mathbf{u}, \quad (1)$$

where $\mathbf{u} = (u_1, u_2, u_3) = (u_k)$ is the displacement vector of any one of the three waves corresponding to the specified wave normal $\mathbf{n} = (n_i)$, $\mathbf{n}^2 = 1$; v is the corresponding phase velocity, and the tensor Λ is expressed in terms of the tensor of elastic moduli of the crystal c_{ijkl} , the density ρ , and $\mathbf{n}$ in the following way: $\Lambda = (\Lambda_{ik}) = \frac{1}{\rho}(c_{ijkl}n_jn_l)$. The velocity v is found from the characteristic equation of the third degree $|v^2 - \Lambda| = 0$. Only in hexagonal crystals does this equation decompose into a linear and a quadratic equation (with respect to v^2) for all directions $\mathbf{n}$. In other crystals such a decomposition is possible only for certain directions $\mathbf{n}$. Thus, in the general case the problem reduces to solving the complete cubic equation, which greatly complicates the study of the properties of elastic waves in crystals.

Since the values of the elastic moduli c_{ijkl} are known, as a rule, with low accuracy ($\sim 10^{-3}$), it is natural to turn to approximate methods for solving the basic equation (1). In work ⁽¹⁾, for this purpose the standard method of perturbation theory was used, as a consequence of which the results are suitable only for $\mathbf{n}$ lying in the immediate vicinity of those directions for which equation (1) is solved exactly. In work ⁽²⁾ a method was presented for the approximate solution of equation (1) for any $\mathbf{n}$, but only for quasi-longitudinal waves, while in ⁽⁵⁾ another method was given, suitable for transverse waves. In the present work an effective general method is set forth for the approximate solution of equation (1) for any specified $\mathbf{n}$ and for all three corresponding waves.

As shown in ⁽³⁾, the tensor Λ for any crystal can be represented in the form

$$\Lambda = a + b(\mathbf{n} \cdot \mathbf{n} + \alpha), \quad a = \frac{1}{2}(\Lambda_c - \mathbf{n}\Lambda\mathbf{n}), \quad b = \frac{1}{2}(3\mathbf{n}\Lambda\mathbf{n} - \Lambda_c), \quad (2)$$

where Λ_c is the trace of the tensor Λ , and $\mathbf{n} \cdot \mathbf{n} = (n_i n_k)$ is a dyad. In this representation the terms $a + b\mathbf{n} \cdot \mathbf{n} = \Lambda^0$ form a tensor of the same structure as for an isotropic medium. The tensor α ($\alpha_c = \mathbf{n}\alpha\mathbf{n} = 0$) characterizes the relative difference of the tensor Λ from Λ^0 and is small in comparison with Λ or Λ^0 . Introduce the vectors $\mathbf{h}$, $\mathbf{u}'$, and the number x by means of the relations $\begin{pmatrix} 2 \\ 3 \end{pmatrix}$

$$\mathbf{h} = \alpha\mathbf{n} = \frac{1}{b}[\mathbf{n}[\Lambda\mathbf{n}, \mathbf{n}]], \quad \mathbf{n}\mathbf{h} = \mathbf{n}\alpha\mathbf{n} = 0; \quad (3)$$

$$\mathbf{u} = \mathbf{n} + \mathbf{u}', \quad \mathbf{u}'\mathbf{n} = 0, \quad (4)$$

$$v^2 = a + bx. \quad (5)$$

Substituting (2)–(5) into (1), we obtain

$$(x - \alpha)\mathbf{u}' = (1 - x)\mathbf{n} + \mathbf{h}. \quad (6)$$

On the other hand, the equation $|v^2 - \Lambda| = 0$ can be transformed covariantly (see (2-4)), with allowance for (2)–(5), to the form

$$x^3 - x^2 - q^2x + \chi^2 - |\alpha| = (x - 1)(x^2 - g^2) - (\mathbf{h}^2 + |\alpha|) = 0, \quad (7)$$

where

$$g^2 = \frac{1}{2}(a^2)_c = \mathbf{h}^2 + \chi^2. \quad (8)$$

For a purely longitudinal wave $[\Lambda\mathbf{n}, \mathbf{n}] = 0$; therefore, according to (3), in this case $|\mathbf{h}| = |\alpha| = 0$. For a quasilonitudinal wave the displacement $\mathbf{u}$ should differ little from $\mathbf{n}$, and therefore v^2 should be close to $\mathbf{n}\Lambda\mathbf{n} = a + b$, which, according to (5), corresponds to $x = 1$. Substituting in (7) $x = 1 + \xi_0$, where $\xi_0 < 1$, we obtain

$$\xi_0 = \frac{\mathbf{h}^2 + |\alpha|}{(1 + \xi_0)^2 - g^2}. \quad (9)$$

From this formula ξ_0 is readily found by iteration:

$$\xi_0^{(k+1)} = \frac{\mathbf{h}^2 + |\alpha|}{(1 + \xi_0^{(k)})^2 - g^2}, \quad \xi_0^{(0)} = 0. \quad (10)$$

Thus we obtain

$$\xi_0^{(1)} = \frac{\mathbf{h}^2 + |\alpha|}{1 - g^2} = \mathbf{h}^2 + |\alpha|, \quad (11)$$

$$\xi_0^{(2)} = \mathbf{h}^2(1 + \chi^2 - \mathbf{h}^2) + |\alpha|(1 + \chi^2 - 3\mathbf{h}^2) \quad (12)$$

and so on. In general, the k -th approximation contains the correct terms up to and including degree $(2k + 1)$ with respect to the components a . In practice the first approximation already proves quite sufficient for most crystals, and the second for almost all crystals.

Denoting the solutions of equation (7) for the quasitransverse waves by $\xi_{\pm}$, we obtain, according to Vieta's formulas, $\xi_0 + \xi_+ + \xi_- = 0$, $(1 + \xi_0)(\xi_+ + \xi_-) + \xi_+ \xi_- = -g^2$, $(1 + \xi_0)\xi_+ \xi_- = |\alpha| - \chi^2$, whence it follows that $\xi_{\pm}$ are the roots of the quadratic equation $\xi^2 + \xi_0 \xi + \xi_0(1 + \xi_0) - g^2 = 0$, i.e.

$$\xi_{\pm} = \frac{1}{2} \left(-\xi_0 \pm \sqrt{4(g^2 - \xi_0) - 3\xi_0^2} \right) = \frac{1}{2} \left(-\xi_0 \pm \sqrt{\xi_0^2 + 4\frac{\chi^2 - |\alpha|}{1 + \xi_0}} \right). \quad (13)$$

This formula, like (9), is exact. Therefore, if ξ_0 has been obtained from (10) in some approximation, then, substituting this value into (13), we find $\xi_{\pm}$ with the same accuracy. It is more convenient, however, to find $\xi_{\pm}$ directly from equation (7) by iteration. In doing so, first, we obtain rational expressions for $\xi_{\pm}$, and second, values of $\xi_{\pm}$ with any degree of accuracy can be obtained independently of the preliminary determination of ξ_0 . For this purpose we write equation (7) in the form

$$(x^2 - \chi^2) = \frac{\mathbf{h}^2 x + |\alpha|}{x - 1}, \quad (14)$$

whence the iterative formula follows

$$\xi_{\pm}^{(k+1)} = \pm\chi - \frac{\mathbf{h}^2 \xi_{\pm}^{(k)} + |\alpha|}{(1 - \xi_{\pm}^{(k)})(\xi_{\pm}^{(k)} \pm \chi)}, \quad \xi_{\pm}^{(0)} = \pm\chi. \quad (15)$$

In particular, the first approximation has the form

$$\xi_{\pm}^{(1)} = \pm\chi - \frac{1}{2\chi}(1 \mp \chi)(\mathbf{h}^2 \chi \pm |\alpha|). \quad (16)$$

* Here $|\mathbf{h}| = \sqrt{\mathbf{h}^2}$ is the length of the vector $\mathbf{h}$, and $|\alpha|$ is the determinant of the matrix α .

Formula (14), like (9), gives, for the k -th approximation, results correct up to and including terms of degree $2k + 1$ with respect to the components α . Thus, with the aid of (5), (10), (13), and (15), we readily obtain the values of the phase velocities of all three waves for any direction $\mathbf{n}$ in an arbitrary crystal with any desired degree of accuracy.

To determine the corresponding displacement vectors, let us turn to formulas (4), (6). Taking x as known and solving (6) covariantly with respect to $\mathbf{u}'$, we obtain, taking (7) into account (see ⁽²⁻⁴⁾),

$$\mathbf{u}' = \frac{(x + \alpha)\mathbf{h} - \mathbf{h}^2 \cdot \mathbf{n}}{x^2 - \kappa^2} = \frac{x\mathbf{h} + [\mathbf{n}[\alpha\mathbf{h}, \mathbf{n}]]}{x^2 - \kappa^2}. \quad (17)$$

For the quasi-longitudinal wave, $x = 1 + \xi_0 \gg \kappa^2$, and therefore from this formula the addition to $\mathbf{n}$ (see (4)) is determined directly; it characterizes the deviation of the wave displacement vector from the direction $\mathbf{n}$. Formula (17) is exact; hence the degree of approximation for $\mathbf{u} = \mathbf{n} + \mathbf{u}'$ is determined by the approximation taken for x . Thus, taking ξ_0 in the first approximation (11), we obtain for the displacement of the quasi-longitudinal wave, according to (4), (17),

$$\begin{aligned} \mathbf{u} = \mathbf{u}_0 = \mathbf{n} + \frac{(1 + \mathbf{h}^2 + |\alpha|)\mathbf{h} - \alpha\mathbf{h} - \mathbf{h}^2 \cdot \mathbf{n}}{(1 + \mathbf{h}^2 + |\alpha|)^2 - \kappa^2} = \\ = \mathbf{n} + (1 + \kappa^2 - \mathbf{h}^2 - |\alpha|)\mathbf{h} + (1 + \kappa^2 - 2\mathbf{h})[\mathbf{n}[\alpha\mathbf{h}, \mathbf{n}]]. \end{aligned} \quad (18)$$

This expression is exact up to and including terms of fourth order in α . In general, taking ξ_0 in the k -th approximation, we obtain $\mathbf{u}_0$ with accuracy up to and including terms of degree $2k + 2$ in α .

For quasi-transverse waves, it is inconvenient to use formula (17), since in this case the denominator $x^2 - \kappa^2$ will be very small or equal to zero, and the addition $\mathbf{u}'$ will considerably exceed the unit vector $\mathbf{n}$ in magnitude. Since we are interested in the *direction* of the displacement vector $\mathbf{u} = \mathbf{u}_\pm$, we may take $\mathbf{u} = C(\mathbf{n} + \mathbf{u}')$ with an arbitrary multiplier C . Bringing the sum $\mathbf{n} + \mathbf{u}'$ to a common denominator and discarding it, we obtain the general exact formula

$$\mathbf{u} = (x^2 - g^2)\mathbf{n} + (x + \alpha)\mathbf{h}. \quad (19)$$

Substituting here the values $x = \xi_\pm$ found from (15), we obtain, with the corresponding accuracy, the directions of the displacement vectors $\mathbf{u}_\pm$ of the quasi-transverse waves. Thus, the relations given above provide a complete and practically effective solution of the problem of finding the velocities and displacements of elastic waves for all directions in any crystals.

Institute of Physics
Academy of Sciences of the BSSR

Received
16 XII 1963

CITED LITERATURE

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