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SOUND VELOCITY ANISOTROPY IN CUBIC CRYSTALS

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ABSTRACT

Simple analytical expressions may be derived for sound velocities in cubic crystals by using lattice harmonics or functions which are invariant under the crystal symmetry operations. These expressions are in good agreement with the exact results for typical crystals such as metallic iron and potassium fluoride.

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The propagation of sound waves in single crystals is governed by a set of three simultaneous linear equations known as the Christoffel equations. [1-3] The characteristic equation relates the sound velocity v to the direction $\underset{\sim}{n}$ of sound wave and to the elastic constants of the crystal. When the direction $\underset{\sim}{n}$ lies along a crystal symmetry axis, simple solutions may be obtained for the sound velocities. In many cases, these simple solutions may be readily reversed so that the measured sound velocities may be used to calculate the elastic constants. However, there are many situations where the solution of the characteristic equation is required for arbitrary crystallographic directions; for example, an argon crystal grown at low temperatures may be inaccessible except for sound velocity measurements. [4,5] For these arbitrary directions, it is advantageous to have simple approximate solutions, preferrably analytical in form.

Many experimental quantities, such as nuclear magnetic resonance (NMR) second moments and sound velocities, are invariant under the crystal symmetry operations, thus they may be expanded in terms of lattice harmonics of the identity representation. These lattice harmonics are specific linear combinations of spherical harmonics which are invariant under the crystal symmetry operations. [6-8] The linear expansions are very convenient for certain experimental quantities such as NMR second moments where it can be rigorously shown that the expansion is limited to only the zeroth, second and fourth order spherical harmonics. [9] However, such limitations may be absent for the sound velocities, thus the linear expansions many converge rather

slowly. In this paper, the simple analytical solutions for sound velocities along the major crystal symmetry axes have been extended to arbitrary directions for cubic crystals. However, we have not restricted ourselves to linear expansions alone. Instead, we have used simple functional forms which are chosen to fit the experimental data exactly along various directions with high crystal symmetry. These approximate solutions have been compared with the exact results, and the agreements are satisfactory.

By choosing the reference or coordinate axes to be coincident with the edges of a cubic cell, then the cubic crystal is characterized by three elastic stiffness constants, c_{11}, c_{12} and c_{44}. The Kelvin-Christoffel stiffnesses are given by [1-3]

$$\Gamma_{ii} = n_i^2(c_{11} - c_{44}) + c_{44} \tag{1}$$

$$\Gamma_{ij} = n_i n_j(c_{12} + c_{44}) \quad \text{for} \quad i \neq j \tag{2}$$

where n_1, n_2 and n_3 are the components of the unit vector $\underset{\sim}{n}$. The sound velocities v are obtained by solving the characteristic equation or determinant $|\Gamma_{ij} - \rho v^2 \delta_{ij}| = 0$ where ρ is the density of the crystal. This equation may be simplified by introducing the dimensionless variables $\lambda = (\rho v^2 - c_{44})/(c_{11} - c_{44})$ and $\beta = (c_{12} + c_{44})/(c_{11} - c_{44})$ so that the eigenvalue λ depends only on a single parameter β characteristic of the cubic crystal:

$$\begin{vmatrix} n_1^2 - \lambda & \beta n_1 n_2 & \beta n_1 n_3 \\ \beta n_1 n_2 & n_2^2 - \lambda & \beta n_2 n_3 \\ \beta n_1 n_3 & \beta n_2 n_3 & n_3^2 - \lambda \end{vmatrix} = 0 \tag{3}$$

On expanding the determinant, we get the cubic equation

$$\lambda^3 - \lambda^2 + P(1-\beta^2)\lambda - Q(1-\beta)^2(1+2\beta) = 0. \qquad (4)$$

where $P = n_1^2n_2^2 + n_2^2n_3^2 + n_3^2n_1^2$ and $Q = n_1^2n_2^2n_3^2$ are fourth and sixth order functions which are invariant under the crystal symmetry operations. These functions are equivalent to the lattice harmonics [6,7] after orthogonalization and normalization; for example, the fourth order lattice harmonic is given by $-(525/16\pi)^{\frac{1}{2}}[P - (1/5)]$. From (3) or (4), the eigenvalues have simple forms when $\underset{\sim}{n}$ is parallel to one of the three major crystal axes, the cubic edge [100], the face diagonal [110], and the body diagonal [111]: [1-3]

$\underset{\sim}{n} \parallel [100]$: $P=0$, $Q=0$, $\lambda_L=1$, $\lambda_T=0,0$.

$\underset{\sim}{n} \parallel [110]$: $P=1/4$, $Q=0$, $\lambda_L=(1+\beta)/2$, $\lambda_T=0$, $(1-\beta)/2$.

$\underset{\sim}{n} \parallel [111]$: $P=1/3$, $Q=1/27$, $\lambda_L=(1+2\beta)/3$, $\lambda_T=(1-\beta)/3$, $(1-\beta)/3$.

The largest eigenvalue λ_L refers to the longitudinal wave whereas the other two eigenvalues λ_T refer to the two transverse or shear waves. It may also be seen from (3) or (4) that $\lambda_T=0$ for one of the transverse waves when $\underset{\sim}{n}$ is perpendicular to one of the cube edges ($Q=0$). Furthermore, simple results may also be obtained when $\underset{\sim}{n}$ is perpendicular to one of the face diagonals. By defining $\lambda = u(1-\beta)$, then (4) may be written as

$$[1-\beta]^2[(u^3 - u^2+Pu-Q) + \beta(-u^3+Pu-2Q)] = 0. \qquad (5)$$

If u is independent of β, then both parentheses in (5) would be zero. Solving $u^3-u^2+Pu-Q=0$ and $-u^3+Pu-2Q=0$ for P and Q, we get

$$P = 2u - 3u^2, \quad Q = u^2(1-2u). \qquad (6)$$

When $\underset{\sim}{n}$ is perpendicular to one of the face diagonals, then $n_1=n_2$ and $n_3^2 = 1 - 2n_1^2$. Thus we have

$$P = 2n_1^2 - 3n_1^4, \quad Q = n_1^4(1 - 2n_1^2). \tag{7}$$

Comparison with (6) indicates that $u=n_1^2$ is one of the solutions. Thus one of the transverse wave eigenvalues is $\lambda_T = n_1^2(1-\beta)$. For $n_1=n_2$, the characteristic equation is obtained by the substitution of (7) into (4):

$$\lambda^3 - \lambda^2 + P(1-\beta^2)(2n_1^2 - 3n_1^4)\lambda - n_1^4(1-2n_1^2)(1-\beta)^2(1+2\beta) = 0.$$

Since one of the solutions is $n_1^2(1-\beta)$, this cubic equation may be factorized into the product of $\lambda - n_1^2(1-\beta)$ and the quadratic equation

$$\lambda^2 - [1+n_1^2(\beta-1)]\lambda - (\beta-1)(2\beta+1)n_1^2(1 - 2n_1^2) = 0. \tag{8}$$

The other two eigenvalues may be obtained by solving (8).

We will now extend these simple solutions to arbitrary directions of $\underset{\sim}{n}$. For the longitudinal wave, the simple function

$$\lambda_L = 1 - 2(1-\beta)P \tag{9}$$

agrees with the eigenvalues for $\underset{\sim}{n}$ along any one of the three major axes (100, 110, 111). The next order correction would be proportional to an invariant function up to the eighth order. This function would be a linear combination of P, Q and P^2. By imposing the condition that this function vanishes when $\underset{\sim}{n}$ is along one of the three major crystal axes, the result is $4P^2-P-3Q$. Thus we have the result

$$\lambda_L = 1 - 2(1-\beta)P + K(4P^2-P-3Q). \tag{10}$$

The constant K will be chosen so that λ_L agrees with the exact value when $\underset{\sim}{n}$ is along the [112] crystal axis (this crystal axis is perpendicular to both a face diagonal and a body diagonal), where we have $n_1^2 = n_2^2 = 1/6$, $n_3^2 = 2/3$, $P = 1/4$, $Q = 1/54$, and

$4P^2-P-3Q = -1/18$. From (8), we get $\lambda_L = [5+\beta+(9-6\beta+33\beta^2)^{\frac{1}{2}}]/12$. Substitution into (10) gives $K = (3/2)\left[1+5\beta-(9-6\beta+33\beta^2)^{\frac{1}{2}}\right]$. Thus we get

$$\lambda_L = 1 - 2(1-\beta)P + (3/2)\left[1+5\beta-(9-6\beta+33\beta^2)^{\frac{1}{2}}\right](4P^2-P-3Q) \qquad (11)$$

for the longitudinal waves.

From (3) or (4), the sum of the three eigenvalues is always unity, hence it is necessary to evaluate λ_T for only one of the transverse waves. We note that $\lambda_T=0$ when $Q=0$ ($\underset{\sim}{n}$ perpendicular to a cube edge) and that $\lambda_T = n_1^2(1-\beta)$ when $n_1=n_2$ ($\underset{\sim}{n}$ perpendicular to a face diagonal). Because of these restrictions, it may not be advantageous to expand λ_T as linear combinations of lattice harmonics or invariant functions. For $\underset{\sim}{n}$ perpendicular to a face diagonal, we get $P^2-3Q = (n_1^2 - 3n_1^4)^2$ from (7), hence we have $n_1^2 = P - (P^2-3Q)^{\frac{1}{2}}$ and it follows that

$$\lambda_T = (1-\beta)\left[P-(P^2-3Q)^{\frac{1}{2}}\right] \qquad (12)$$

This relationship is also exact for $\underset{\sim}{n}$ perpendicular to a cube edge ($\lambda_T=0$ when $Q=0$). We note that from (7), n_1^2 may also take other forms. For example, we may also write $n_1^2=(2P^2-6Q)/(P-9Q)$. However, the expression $\lambda_T = (1-\beta)(2P^2-6Q)/(P-9Q)$ will not vanish for $Q=0$.

The anisotropy (or the variation with the direction of the sound wave) of the eigenvalues depends only on the dimensionless parameter β. For $\beta=1$, the three eigenvalues are $\lambda=1,0,0$ for any direction; that is, there is no anisotropy for the sound velocities. Usually (although not always), we have $\beta<1$ for ionic crystals and $\beta>1$ for metals; the extreme values are $\beta=0.19$

for SnTe and β=6 for metallic sodium. [2, 10] Typical values are β=2.1866 for metallic iron (c_{11}=23.30, c_{12}=13.92 and c_{44}=11.62 in units of 10^{11} dynes/cm^2) and β=0.523 for potassium fluoride (c_{11}=6.58, c_{12}=1.49 and c_{44}=1.28). The exact eigenvalues for these crystals are shown in Fig. 1 and Fig. 2 as the solid lines for $\underset{\sim}{n}$ in the (100), (110) and (111) crystal planes by solving (3) or (4) numerically. The points in the figures are the approximate eigenvalues obtained from the analytical expressions (11) and (12) for the longitudinal and transverse waves. For all orientations of the sound wave direction $\underset{\sim}{n}$, the agreement is quite good between the exact and the approximate eigenvalues.

In conclusion, it may be seen that simple analytical expressions may be used with good accuracy for sound velocities in cubic crystals. These expressions are based on the lattice harmonics or functions which are invariant under the symmetry operations of the crystal. Whereas linear expansions can be used for the longitudinal waves, other functional forms may be necessary for the transverse waves because of the "cross-overs" of the two branches. These simple results may be useful for fitting experimental data of materials of unknown orientations crystallized at low temperatures or for the inversions of sound velocity data to obtain the elastic constants. [4,5]

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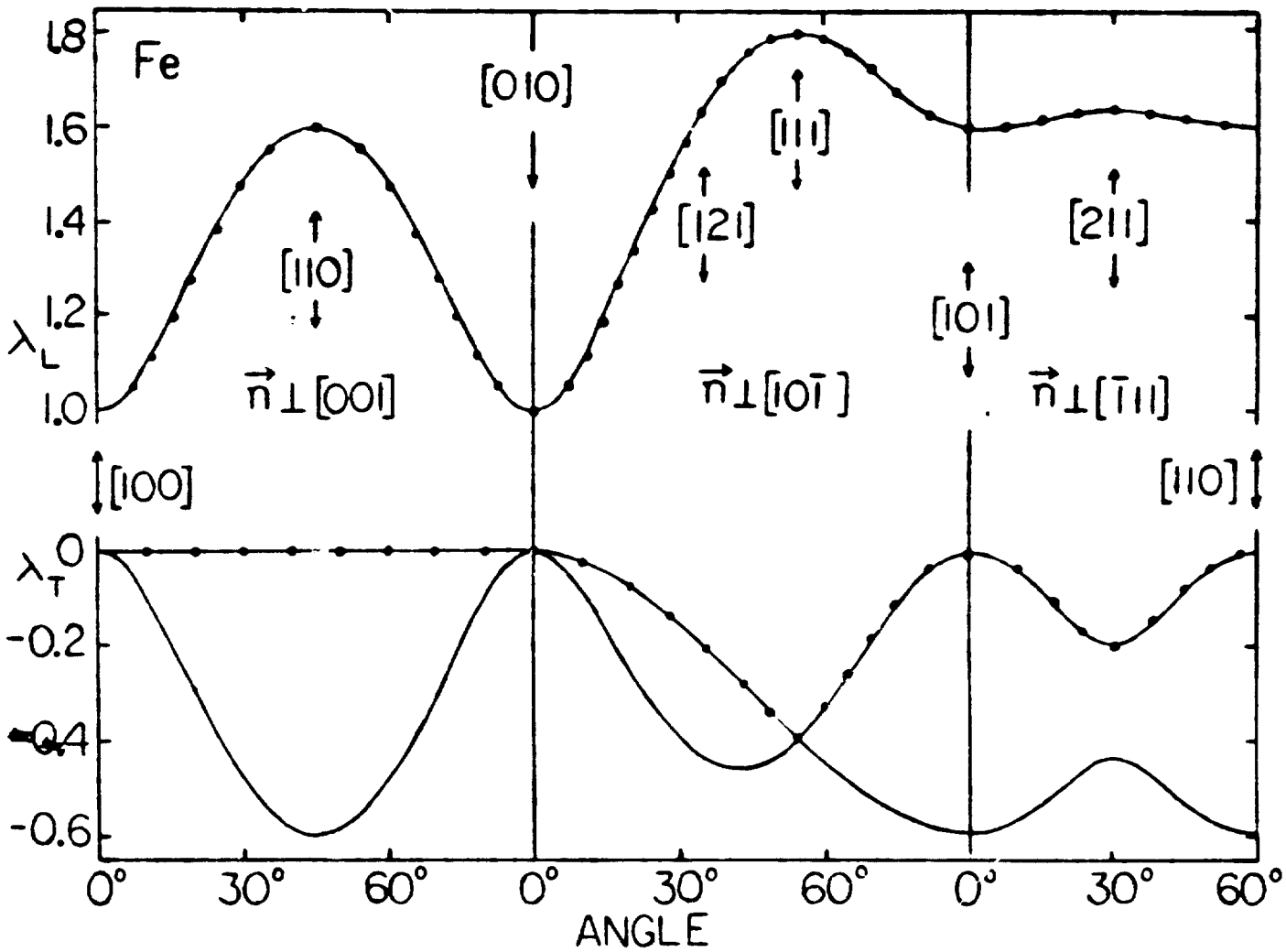
FIGURE CAPTIONS

Fig. 1. Eigenvalues λ_L and λ_T of the longitudinal and transverse waves for metallic iron (β=2.1866) when $\underset{\sim}{n}$ is in the (100), (110) and (111) crystal planes. Solid lines are the exact values from (4). The points are the approximate values from the analytical expressions (11) and (12).

Fig. 2. Eigenvalues λ_L and λ_T of the longitudinal and transverse waves for potassium fluoride (β=0.523) when $\underset{\sim}{n}$ is in the (100), (110) and (111) crystal planes. Solid lines are the exact values from (4). The points are the approximate values from the analytical expressions (11) and (12).



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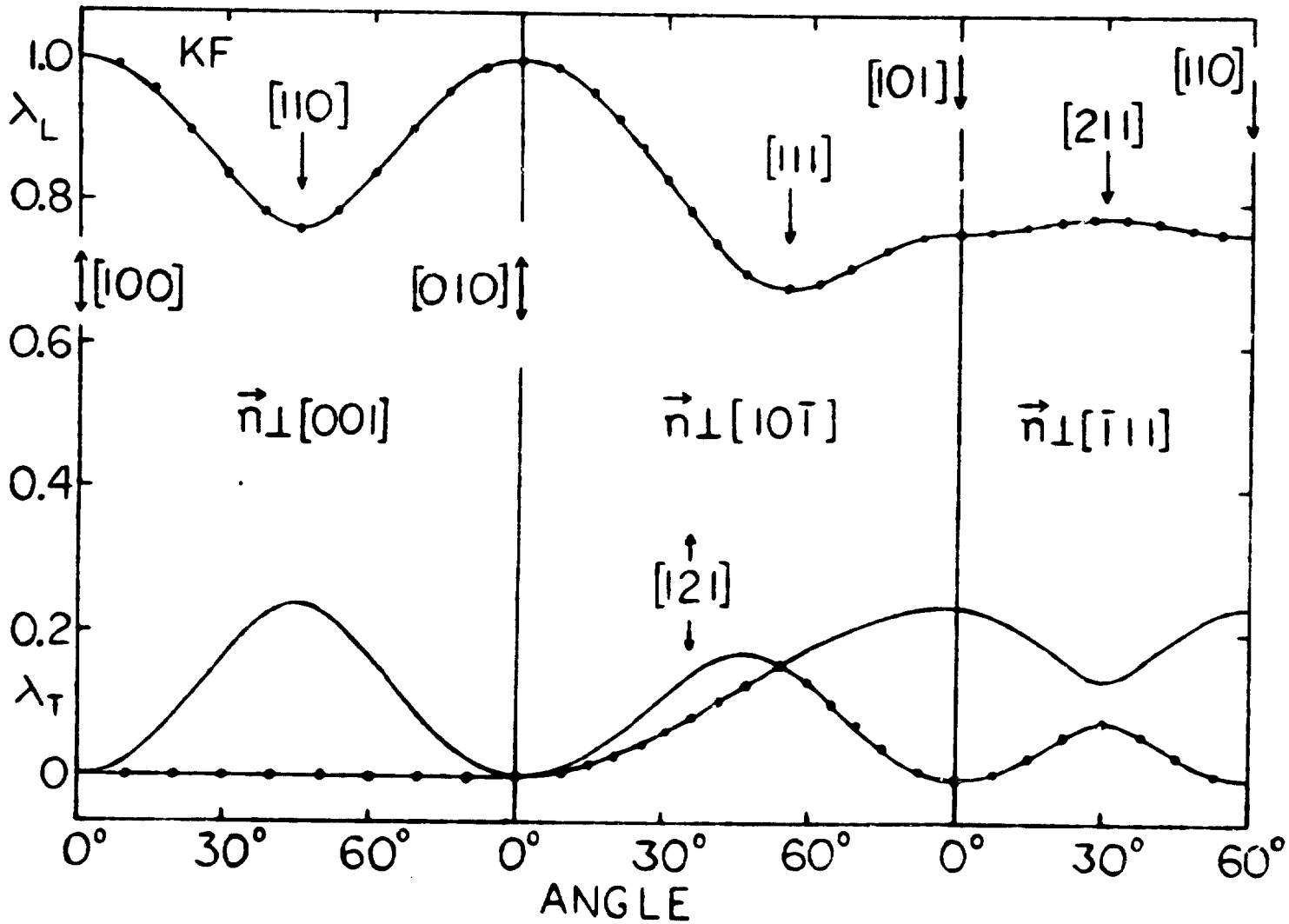

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