*International Tables for Crystallography* (2006). Vol. D, Section 1.3.4.4, pp. 86–87.



## 1.3.4. Propagation of elastic waves in continuous media – dynamic elasticity

### 1.3.4.1. *Introduction*

The elastic properties of materials have been considered in the preceding section in the static state and the elastic constants have been defined in terms of the response of the material to particular static forces. It is effectively the way the elastic constants have been measured in the past, although the measurements could not be very precise. A way of proceeding frequently used now is to excite a mechanical wave in the crystal and measure its propagation velocity or the wavelength associated with a particular frequency. One method consists in sending a train of ultrasonic waves through the crystal; one uses a pulse generator and a piezoelectric transducer glued to the crystal. The elapsed time between the emission of the train of waves and its reception after reflection from the rear face of the sample is then measured. Another method involves producing a system of standing waves after reflection at the inner surface of the crystal and determining the set of resonance frequencies. The experimental techniques will be described in Section 1.3.4.6.

The purpose of the next sections is to establish relations between the wavelength – or the velocity of propagation – and the elastic constants.

### 1.3.4.2. *Equation of propagation of a wave in a material*

Consider the propagation of a wave in a continuous medium. The elongation of each point will be of the form

$$\mathbf{u} = \mathbf{u_0} \exp(2\pi i \nu t) \exp(-2\pi i \mathbf{q} \cdot \mathbf{r}), \qquad (1.3.4.1)$$

where $\nu$ is the frequency and $\mathbf{q}$ is the wavevector. The velocity of propagation of the wave is

$$V = \nu / q. \qquad (1.3.4.2)$$

We saw in Section 1.3.3.6 that the equilibrium condition is

$$c_{ijkl} \frac{\partial^2 u_k}{\partial x_l \partial x_j} + \rho F_i = 0.$$

Here the only volume forces that we must consider are the inertial forces:

$$c_{ijkl} \frac{\partial^2 u_k}{\partial x_l \partial x_j} = \rho \frac{\partial^2 x_i}{\partial t^2}. \qquad (1.3.4.3)$$

The position vector of the point under consideration is of the form

$$\mathbf{r} = \mathbf{r}_0 + \mathbf{u},$$

where only $\mathbf{u}$ depends on the time and $\mathbf{r}_0$ defines the mean position. Equation (1.3.4.3) is written therefore

$$c_{ijkl} \frac{\partial^2 u_k}{\partial x_l \partial x_j} = \rho \frac{\partial^2 u_i}{\partial t^2}. \qquad (1.3.4.4)$$

Replacing $\mathbf{u}$ by its value in (1.3.4.1), dividing by $-4\pi^2$ and using orthonormal coordinates, we get

$$c_{ijkl} u_k q_j q_l = \rho \nu^2 u_i. \qquad (1.3.4.5)$$

It can be seen that, for a given wavevector, $\rho\nu^2$ appears as an eigenvalue of the matrix $c_{ijkl} u_k q_j q_l$ of which the vibration vector $\mathbf{u}$ is an eigenvector. This matrix is called the dynamical matrix, or *Christoffel matrix*. In order that the system (1.3.4.5) has a solution other than a trivial one, it is necessary that the associated determinant be equal to zero. It is called the Christoffel determinant and it plays a fundamental role in the study of the propagation of elastic waves in crystals.

Let $\alpha_1, \alpha_2, \alpha_3$ be the direction cosines of the wavevector $\mathbf{q}$. The components of the wavevector are

$$q_i = q \alpha_i.$$

With this relation and (1.3.4.2), the system (1.3.4.5) becomes

$$c_{ijkl} u_k \alpha_j \alpha_l = \rho \nu^2 u_i. \qquad (1.3.4.6)$$

Putting

$$\Gamma_{ik} = c_{ijkl} \alpha_j \alpha_l \qquad (1.3.4.7)$$

in (1.3.4.6), the condition that the Christoffel determinant is zero can be written

$$\Delta\left(\Gamma_{ik} - \rho \nu^2 \delta_{ik}\right) = 0. \qquad (1.3.4.8)$$

On account of the intrinsic symmetry of the tensor of elastic stiffnesses, the matrix $\Gamma_{ik}$ is symmetrical.

If we introduce into expression (1.3.4.7) the elastic stiffnesses with two indices [equation (1.3.3.6)], we find, for instance, for $\Gamma_{11}$ and $\Gamma_{12}$

$$\begin{aligned} \Gamma_{11} &= c_{11}(\alpha_1)^2 + c_{66}(\alpha_2)^2 + c_{55}(\alpha_3)^2 + 2c_{16}\alpha_1\alpha_2 \\ &\quad + 2c_{15}\alpha_1\alpha_3 + 2c_{56}\alpha_2\alpha_3 \\ \Gamma_{12} &= c_{16}(\alpha_1)^2 + c_{26}(\alpha_2)^2 + c_{45}(\alpha_3)^2 + (c_{12} + c_{66})\alpha_1\alpha_2 \\ &\quad + (c_{14} + c_{56})\alpha_1\alpha_3 + (c_{46} + c_{25})\alpha_2\alpha_3. \end{aligned}$$

The expression for the effective value, $c^e_{ijkl}$, of the 'stiffened' elastic stiffness in the case of piezoelectric crystals is given in Section 2.4.2.2.

### 1.3.4.3. *Dynamic elastic stiffnesses*

Equation (1.3.4.7) may be written

$$\Gamma_{ik} = \sum_{j \neq l} \left[c_{ijkl} + c_{ilkj}\right] \alpha_j \alpha_l.$$

This shows that in a dynamic process only the sums $[c_{ijkl} + c_{ilkj}]$ can be measured and not $c_{ijkl}$ and $c_{ilkj}$ separately. On the contrary, $c_{ijij}$ can be measured directly. In the cubic system therefore, for instance, $c_{1122}$ is determined from the measurement of $[c_{1122} + c_{1221}]$ on the one hand and from that of $c_{1221}$ on the other hand.

### 1.3.4.4. *Polarization of the elastic waves*

The Christoffel determinant has three roots and the Christoffel matrix, being Hermitian with real coefficients, has three real eigenvalues and three orthogonal eigenvectors. The wavevector $\mathbf{q}$, therefore, encompasses three waves with vibration vectors $\mathbf{u}_1$, $\mathbf{u}_2$, $\mathbf{u}_3$ which are perpendicular to one another. In the general case, there is no particular angular relationship between the vibration vectors (or polarization vectors). However, if the latter are parallel to certain symmetry directions in the crystal, one of the vibration vectors is along this direction. The corresponding

Table 1.3.3.3. *Relations between elastic coefficients in isotropic media*

| Coefficient | In terms of $\mu$ and $\lambda$ | In terms of $\mu$ and $\nu$ | In terms of $c_{11}$ and $c_{12}$ |
|---|---|---|---|
| $c_{11}$ | $2\mu + \lambda$ | $2\mu(1-\nu)/(1-2\nu)$ | $c_{11}$ |
| $c_{12}$ | $\lambda$ | $2\mu\nu(1-2\nu)$ | $c_{12}$ |
| $c_{44} = 1/s_{44}$ | $\mu$ | $\mu$ | $(c_{11} - c_{12})/2$ |
| $E = 1/s_{11}$ | $\mu(2\mu + 3\lambda)/(\mu + \lambda)$ | $2\mu(1+\nu)$ | See Section 1.3.3.2.3 |
| $s_{12}$ | $-\lambda/[2\mu(2\mu + 3\lambda)]$ | $-\nu/[2\mu(1+\nu)]$ | See Section 1.3.3.2.3 |
| $\kappa$ | $3/(2\mu + 3\lambda)$ | $3(1-2\nu)/[2\mu(1+\nu)]$ | $3/(c_{11} + 2c_{12})$ |
| $\nu = -s_{12}/s_{11}$ | $\lambda/[2(2\mu + 3\lambda)]$ | $\nu$ | $c_{11}/(c_{11} + c_{12})$ |

wave is called longitudinal. The two other waves have their polarization direction perpendicular to the wavevector and are thus transverse. If one of the polarization vectors is almost parallel to the wavevector, which often happens, then one speaks of the vibration as being quasi-longitudinal.

1.3.4.5. *Relation between velocity of propagation and elastic stiffnesses*

We shall limit ourselves to cubic, hexagonal and tetragonal crystals and consider particular cases.

1.3.4.5.1. *Cubic crystals*

(i) *The wavevector is parallel to [100]*. The Christoffel determinant reduces to

$$\begin{pmatrix} c_{11} - \rho v^2 & 0 & 0 \\ 0 & c_{44} - \rho v^2 & 0 \\ 0 & 0 & c_{44} - \rho v^2 \end{pmatrix} = 0.$$

The three solutions are given in Table 1.3.4.1. These results are valid for a wave propagating in any direction in an isotropic medium.

(ii) *The wavevector is parallel to [110]*. The direction cosines of the wavevector are $1/\sqrt{2}$, $1/\sqrt{2}$, 0. The Christoffel determinant assumes the form

$$\begin{pmatrix} \frac{1}{2}(c_{11} + c_{44}) - \rho v^2 & \frac{1}{2}(c_{12} + c_{44}) & 0 \\ \frac{1}{2}(c_{12} + c_{44}) & \frac{1}{2}(c_{11} + c_{44}) - \rho v^2 & 0 \\ 0 & 0 & c_{44} - \rho v^2 \end{pmatrix} = 0.$$

The three solutions are given in Table 1.3.4.2.

(iii) *The wavevector is parallel to [111]*. The Christoffel determinant assumes the form

$$\begin{pmatrix} c_{11} + 2c_{44} - \rho v^2 & c_{12} + c_{44} & c_{12} + c_{44} \\ c_{12} + c_{44} & c_{11} + 2c_{44}) - \rho v^2 & c_{12} + c_{44} \\ c_{12} + c_{44} & c_{12} + c_{44} & c_{44} - \rho v^2 \end{pmatrix} = 0.$$

The solutions are given in Table 1.3.4.3.

1.3.4.5.2. *Hexagonal crystals*

In hexagonal crystals, there are five independent elastic stiffnesses, $c_{11}$, $c_{33}$, $c_{12}$, $c_{13}$, $c_{44}$ and $c_{66} = (c_{11} - c_{12})/2$ (Section 1.1.4.10.4).

(i) *The wavevector is parallel to [001]*. The Christoffel determinant reduces to

$$\begin{pmatrix} c_{44} - \rho v^2 & 0 & 0 \\ 0 & c_{44} - \rho v^2 & 0 \\ 0 & 0 & c_{33} - \rho v^2 \end{pmatrix} = 0.$$

The solutions are given in Table 1.3.4.4.

(ii) *The wavevector is parallel to [100]*. The Christoffel determinant readily reduces to

$$\begin{pmatrix} c_{11} - \rho v^2 & 0 & 0 \\ 0 & c_{66} - \rho v^2 & 0 \\ 0 & 0 & c_{44} - \rho v^2 \end{pmatrix} = 0.$$

The three solutions are given in Table 1.3.4.5.

1.3.4.5.3. *Tetragonal crystals (classes* $4mm$, $\bar{4}2m$, $4/mmm$*)*

In tetragonal crystals, there are six independent elastic stiffnesses, $c_{11}$, $c_{33}$, $c_{12}$, $c_{13}$, $c_{44}$ and $c_{66}$ (Section 1.1.4.10.4).

(i) *The wavevector is parallel to [001]*. The Christoffel determinant reduces to

$$\begin{pmatrix} c_{44} - \rho v^2 & 0 & 0 \\ 0 & c_{44} - \rho v^2 & 0 \\ 0 & 0 & c_{33} - \rho v^2 \end{pmatrix} = 0.$$

The three solutions are given in Table 1.3.4.6.

(ii) *The wavevector is parallel to [100]*. The Christoffel determinant reduces to

$$\begin{pmatrix} c_{11} - \rho v^2 & 0 & 0 \\ 0 & c_{66} -^2 \rho v^2 & 0 \\ 0 & 0 & c_{44} -^2 \rho v^2 \end{pmatrix} = 0.$$

The three solutions are given in Table 1.3.4.7.

Table 1.3.4.1. *Velocity of propagation when the wavevector is parallel to [100] (cubic crystals)*

| Velocity of propagation | Polarization vector | Nature of the wave |
|---|---|---|
| $v_{\parallel} = \sqrt{c_{11}/\rho}$ | [100] | Longitudinal |
| $v_{\perp} = \sqrt{c_{44}/\rho}$ | [010] | Transverse |
| $v_{\perp} = \sqrt{c_{44}/\rho}$ | Any vector normal to [100] | Transverse |

Table 1.3.4.2. *Velocity of propagation when the wavevector is parallel to [110] (cubic crystals)*

| Velocity of propagation | Polarization vector | Nature of the wave |
|---|---|---|
| $v_{\parallel} = \sqrt{[c_{44} + \frac{1}{2}(c_{11} + c_{12})]/\rho}$ | [110] | Longitudinal |
| $v_{\perp} = \sqrt{\frac{1}{2}(c_{11} - c_{12})/\rho}$ | [1$\bar{1}$0] | Transverse |
| $v_{\perp} = \sqrt{c_{44}/\rho}$ | [001] | Transverse |

Table 1.3.4.3. *Velocity of propagation when the wavevector is parallel to [111] (cubic crystals)*

| Velocity of propagation | Polarization vector | Nature of the wave |
|---|---|---|
| $v_{\parallel} = \sqrt{(c_{11} + 2c_{12} + 4c_{44})/3\rho}$ | [111] | Longitudinal |
| $v_{\perp} = \sqrt{(c_{11} - c_{12} + c_{44})/3\rho}$ | Any vector normal to [111] | Transverse |

Table 1.3.4.4. *Velocity of propagation when the wavevector is parallel to [001] (hexagonal crystals)*

| Velocity of propagation | Polarization vector | Nature of the wave |
|---|---|---|
| $v_{\parallel} = \sqrt{c_{33})/\rho}$ | [100] | Longitudinal |
| $v_{\perp} = \sqrt{c_{44}/\rho}$ | Any vector normal to [001] | Transverse |

Table 1.3.4.5. *Velocity of propagation when the wavevector is parallel to [100] (hexagonal crystals)*

| Velocity of propagation | Polarization vector | Nature of the wave |
|---|---|---|
| $v_{\parallel} = \sqrt{c_{11}/\rho}$ | [100] | Longitudinal |
| $v_{\perp} = \sqrt{c_{66}/\rho}$ | [010] | Transverse |
| $v_{\perp} = \sqrt{c_{44}/\rho}$ | [001] | Transverse |

Table 1.3.4.6. *Velocity of propagation when the wavevector is parallel to [001] (tetragonal crystals)*

| Velocity of propagation | Polarization vector | Nature of the wave |
|---|---|---|
| $v_{\parallel} = \sqrt{c_{33}/\rho}$ | [100] | Longitudinal |
| $v_{\perp} = \sqrt{c_{44}/\rho}$ | [010] | Transverse |
| $v_{\perp} = \sqrt{c_{44}/\rho}$ | [001] | Transverse |

Table 1.3.4.7. *Velocity of propagation when the wavevector is parallel to [100] (tetragonal crystals)*

| Velocity of propagation | Polarization vector | Nature of the wave |
|---|---|---|
| $v_{\parallel} = \sqrt{c_{11}/\rho}$ | [100] | Longitudinal |
| $v_{\perp} = \sqrt{c_{66}/\rho}$ | [010] | Transverse |
| $v_{\perp} = \sqrt{c_{44}/\rho}$ | [001] | Transverse |



references