International Tables for Crystallography (2006). Vol. D, Section 1.3.7.5, pp. 96–97.

$$\rho u_1'' = \mathrm{d}T_{11}/\mathrm{d}X_1$$
$$\rho u_2'' = \mathrm{d}T_{21}/\mathrm{d}X_1$$
$$\rho u_3'' = \mathrm{d}T_{31}/\mathrm{d}X_1.$$

If we retain only terms up to the quadratic order in the displacement gradients, we obtain the following equations of motion:

$$\begin{aligned}\rho u_1'' &= c_{11}\frac{\partial^2 u_1}{\partial X_1^2} + [3c_{11}+c_{111}]\frac{\partial u_1}{\partial X_1}\frac{\partial^2 u_1}{\partial X_1^2}\\ &\quad + (c_{11}+c_{166})\left[\frac{\partial u_2}{\partial X_1}\frac{\partial^2 u_2}{\partial X_1^2} + \frac{\partial u_3}{\partial X_1}\frac{\partial^2 u_3}{\partial X_1^2}\right]\\ \rho u_2'' &= c_{44}\frac{\partial^2 u_2}{\partial X_1^2} + (c_{11}+c_{166})\left[\frac{\partial u_1}{\partial X_1}\frac{\partial^2 u_2}{\partial X_1^2} + \frac{\partial u_2}{\partial X_1}\frac{\partial^2 u_1}{\partial X_1^2}\right]\\ \rho u_3'' &= c_{44}\frac{\partial^2 u_3}{\partial X_1^2} + (c_{11}+c_{166})\left[\frac{\partial u_1}{\partial X_1}\frac{\partial^2 u_3}{\partial X_1^2} + \frac{\partial u_3}{\partial X_1}\frac{\partial^2 u_1}{\partial X_1^2}\right],\end{aligned} \qquad (1.3.7.9)$$

which are identical to (1.3.7.7) if we put

$$c_{11} = \lambda + 2\mu; \quad c_{44} = \mu; \quad c_{111} = 2(l+2m); \quad c_{166} = m.$$

1.3.7.4. *Harmonic generation*

The coordinates in the medium free of stress are denoted either a or $\bar{X}$. The notation $\bar{X}$ is used when we have to discriminate the natural configuration, $\bar{X}$, from the initial configuration X. Here, the process that we describe refers to the propagation of an elastic wave in a medium free of stress (natural state) and the coordinates will be denoted a_i.

Let us first examine the case of a pure longitudinal mode, *i.e.*

$$u_1 = u_1(a_1, t); \quad u_2 = u_3 = 0.$$

The equations of motion, (1.3.7.7) and (1.3.7.9), reduce to

$$\rho u_1'' = (\lambda+2\mu)\frac{\partial^2 u_1}{\partial a_1^2} + [3(\lambda+2\mu)+2(l+2m)]\frac{\partial u_1}{\partial a_1}\frac{\partial^2 u_1}{\partial a_1^2}$$

for an isotropic medium or

$$\rho u_1'' = c_{11}\frac{\partial^2 u_1}{\partial a_1^2} + [3c_{11}+c_{166}]\frac{\partial u_1}{\partial a_1}\frac{\partial^2 u_1}{\partial a_1^2}$$

for a cubic crystal (most symmetrical groups) when a pure longitudinal mode is propagated along [100].

For both cases, we have a one-dimensional problem; (1.3.7.7) and (1.3.7.9) can therefore be written

$$\rho u_1'' = K_2\frac{\partial^2 u_1}{\partial a_1^2} + [3K_2+K_3]\frac{\partial u_1}{\partial a_1}\frac{\partial^2 u_1}{\partial a_1^2}. \qquad (1.3.7.10)$$

The same equation is also valid when a pure longitudinal mode is propagated along [110] and [111], with the following correspondence:

$$[100]\ K_2 = c_{11}, \quad K_3 = c_{111}$$
$$[110]\ K_2 = \frac{c_{11}+c_{12}+2c_{44}}{2}, \quad K_3 = \frac{c_{111}+3c_{112}+12c_{166}}{4}$$
$$[111]\ K_2 = \frac{c_{11}+2c_{12}+4c_{44}}{3},$$
$$K_3 = \frac{c_{111}+6c_{112}+12c_{144}+24c_{166}+2c_{123}+16c_{456}}{9}.$$

Let us assume that $K_3 \ll K_2$; a perturbation solution to (1.3.7.10) is

$$u = u^0 + u^1,$$

where $u^1 \ll u^0$ with

$$u^0 = A\sin(ka-\omega t) \qquad (1.3.7.11)$$
$$u^1 = Ba\sin 2(ka-\omega t) + Ca\cos 2(ka-\omega t). \qquad (1.3.7.12)$$

If we substitute the trial solutions into (1.3.7.10), we find after one iteration the following approximate solution:

$$u = A\sin(ka-\omega t) - \frac{(kA)^2(3K_2+K_3)}{8\rho c^2}a\cos 2(ka-\omega t),$$

which involves second-harmonic generation.

If additional iterations are performed, higher harmonic terms will be obtained. A well known property of the first-order nonlinear equation (1.3.7.10) is that its solutions exhibit discontinuous behaviour at some point in space and time. It can be seen that such a discontinuity would appear at a distance from the origin given by (Breazeale, 1984)

$$L = -2\frac{(K_2)^2}{3K_2+K_3}\rho\omega u_0',$$

where u_0' is the initial value for the particle velocity.

1.3.7.5. *Small-amplitude waves in a strained medium*

We now consider the propagation of small-amplitude elastic waves in a homogeneously strained medium. As defined previously, $\bar{X}$ or a are the coordinates in the natural or unstressed state. X are the coordinates in the initial or homogeneously strained state. $u_i = x_i - X_i$ are the components of displacement from the initial state due to the wave.

Starting from (1.3.7.4), we get

$$T_{ij} = \frac{\rho_0}{J}\alpha_{ik}\alpha_{jl}\frac{\partial U}{\partial S_{kl}}.$$

Its partial derivative is

$$\frac{\partial T_{ij}}{\partial x_j} = \frac{1}{J}\frac{\partial}{\partial X_k}\left[\rho_0\alpha_{il}\frac{\partial U}{\partial S_{kl}}\right].$$

If we expand the state function about the initial configuration, it follows that

$$\rho_0 U(X_k, S_{ij}) = \rho_0 U(X_k) + c_{ij}S_{ij} + \tfrac{1}{2}c_{ijkl}S_{ij}S_{kl} + \tfrac{1}{6}c_{ijklmn}S_{ij}S_{kl}S_{mn} + \ldots.$$

The linearized stress derivatives become

$$\frac{\partial T_{ij}}{\partial x_j} = \left[c_{jl}\delta_{ik} + c_{ijkl}\right]\frac{\partial^2 x_k}{\partial X_j \partial X_l}.$$

If we let $D_{ijkl} = \left[c_{jl}\delta_{ik} + c_{ijkl}\right]$, the equation of motion in the initial state is

$$\rho_0 u_i'' = D_{jkli}\frac{\partial^2 u_k}{\partial X_j \partial X_l}. \qquad (1.3.7.13)$$

The coefficients D_{ijkl} do not present the symmetry of the coefficients c_{ijkl} except in the natural state where D_{ijkl} and c_{ijkl} are equal.

The simplest solutions of the equation of motion are plane waves. We now assume plane sinusoidal waves of the form

$$u_i = A_i\exp[i(\omega t - \mathbf{k}\cdot\mathbf{X})], \qquad (1.3.7.14)$$

where $\mathbf{k}$ is the wavevector.

Substitution of (1.3.7.14) into (1.3.7.13) results in

$$\rho_0\omega^2 A_j = D_{ijkl}k_j k_l A_k$$

Table 1.3.7.1. *Relationships between ρW^2, its pressure derivatives and the second- and third-order elastic constants*

Propagation	Polarization	$(\bar{\rho}_0 W^2)_0$	$\partial(\bar{\rho}_0 W^2)_0/\partial p$
[100]	[100]	$\bar{c}_{11}$	$-1-(2\bar{c}_{11}+\Gamma_{1111})/3\bar{\kappa}$
[100]	[010]	$\bar{c}_{44}$	$-1-(2\bar{c}_{44}+\Gamma_{2323})/3\bar{\kappa}$
[110]	[110]	$(\bar{c}_{11}+\bar{c}_{12}+2\bar{c}_{44})/2$	$-1-\big(\bar{c}_{11}+\bar{c}_{12}+2\bar{c}_{44}+0.5[\Gamma_{1111}+\Gamma_{1122}+\Gamma_{2323}]\big)/3\bar{\kappa}$
[110]	[1$\bar{1}$0]	$(\bar{c}_{11}-\bar{c}_{12}+\bar{c}_{44})/3$	$-1-\big(\bar{c}_{11}-\bar{c}_{11}+0.5[\Gamma_{1111}-\Gamma_{1122}]\big)/3\bar{\kappa}$
[110]	[001]	$\bar{c}_{44}$	$-1-(2\bar{c}_{44}+\Gamma_{2323})/3\bar{\kappa}$
[111]	[111]	$(\bar{c}_{11}+2\bar{c}_{12}+4\bar{c}_{44})/3$	$-1-\big(2\bar{c}_{11}+4\bar{c}_{12}+8\bar{c}_{14}+[\Gamma_{1111}+2\Gamma_{1122}+4\Gamma_{2323}]\big)/9\bar{\kappa}$
[111]	[1$\bar{1}$0]	$(\bar{c}_{11}-\bar{c}_{12}+\bar{c}_{44})/3$	$-1-\big(2\bar{c}_{11}-2\bar{c}_{12}+2\bar{c}_{14}+[\Gamma_{1111}-\Gamma_{1122}+\Gamma_{2323}]\big)/9\bar{\kappa}$

or

$$\rho_0\omega^2 A_j = \Delta_{jk} A_k$$

with $\Delta_{jk} = D_{ijkl} k_j k_l$.

The quantities $\rho_0\omega^2 A_j$ and A are, respectively, the *eigenvalues* and *eigenvectors of the matrix* Δ_{jk}. Since Δ_{jk} is a real symmetric matrix, the eigenvalues are real and the eigenvectors are orthogonal.

1.3.7.6. *Experimental determination of third- and higher-order elastic constants*

The main experimental procedures for determining the third- and higher-order elastic constants are based on the measurement of stress derivatives of ultrasonic velocities and on harmonic generation experiments. Hydrostatic pressure, which can be accurately measured, has been widely used; however, the measurement of ultrasonic velocities in a solid under hydrostatic pressure cannot lead to the whole set of third-order elastic constants, so uniaxial stress measurements or harmonic generation experiments are then necessary.

In order to interpret wave-propagation measurements in stressed crystals, Thurston (1964) and Brugger (1964) introduced the concept of natural velocity with the following comments:

'According to equation of motion, the wave front is a material plane which has unit normal **k** in the natural state; a wave front moves from the plane $\mathbf{k}\cdot\mathbf{a}=\mathbf{0}$ to the plane $\mathbf{k}\cdot\mathbf{a}=\mathbf{L_0}$ in the time L_0/W. Thus W, *the natural velocity*, is the wave speed referred to natural dimensions for propagation normal to a plane of natural normal **k**.

In a typical ultrasonic experiment, plane waves are reflected between opposite parallel faces of a specimen, the wave fronts being parallel to these faces. One ordinarily measures a repetition frequency F, which is the inverse of the time required for a round trip between the opposite faces.'

Hence

$$W = 2L_0F.$$

In most experiments, the third-order elastic constants and higher-order elastic constants are deduced from the stress derivatives of $\bar{\rho}_0W^2$. For instance, Table 1.3.7.1 gives the expressions for $(\bar{\rho}_0W^2)_0$ and $\partial(\bar{\rho}_0W^2)_0/\partial p$ for a cubic crystal. These quantities refer to the natural state free of stress. In this table, p denotes the hydrostatic pressure and the Γ_{ijkl}'s are the following linear combinations of third-order elastic constants:

$$\Gamma_{1111} = \bar{c}_{111} + 2\bar{c}_{111}$$
$$\Gamma_{1122} = 2\bar{c}_{112} + \bar{c}_{123}$$
$$\Gamma_{2323} = \bar{c}_{144} + 2\bar{c}_{166}.$$

1.3.8. Glossary

$\mathbf{e}_i$	covariant basis vector
A^T	transpose of matrix A
u_i	components of the displacement vector
S_{ij}	components of the strain tensor
S_α	components of the strain Voigt matrix
T_{ij}	components of the stress tensor
T_α	components of the stress Voigt matrix
p	pressure
$\boldsymbol{\nu}$	normal stress
$\boldsymbol{\tau}$	shear stress
s_{ijkl}	second-order elastic compliances
$s_{\alpha\beta}$	reduced second-order elastic compliances
$(s_{ijkl})^\sigma$	adiabatic second-order elastic compliances
s_{ijklmn}	third-order elastic compliances
c_{ijkl}	second-order elastic stiffnesses
$(c_{ijkl})^\sigma$	adiabatic second-order elastic stiffnesses
$c_{\alpha\beta}$	reduced second-order elastic stiffnesses
c_{ijklmn}	third-order elastic stiffnesses
ν	Poisson's ratio
E	Young's modulus
κ	bulk modulus (volume compressibility)
λ, μ	Lamé constants
Θ	temperature
c^S	specific heat at constant strain
ρ	volumic mass
Θ_D	Debye temperature
k_B	Boltzmann constant
U	internal energy
F	free energy

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