International Tables for Crystallography (2013). Vol. D, Section 1.3.7.3, pp. 95–97.

$$\begin{aligned}\Phi = &\tfrac{1}{2}c_{11}\big[(S_{11})^2+(S_{22})^2+(S_{33})^2\big]+c_{12}\big[S_{11}S_{22}+S_{22}S_{33}+S_{33}S_{11}\big]\\ &+c_{44}[(S_{12})^2+(S_{21})^2+(S_{23})^2+(S_{32})^2+(S_{31})^2+(S_{13})^2]\\ &+c_{111}\big[(S_{11})^3+(S_{22})^3+(S_{33})^3\big]\\ &+c_{112}\big[(S_{11})^2(S_{22}+S_{33})+(S_{22})^2(S_{33}+S_{11})\\ &+(S_{33})^2(S_{11}+S_{22})\big]\\ &+\tfrac{1}{2}c_{144}\{S_{11}[(S_{23})^2+(S_{32})^2]+S_{22}[(S_{31})^2+(S_{13})^2]\\ &+S_{33}[(S_{12})^2+(S_{21})^2]\}\\ &+\tfrac{1}{2}c_{166}\{\big[(S_{12})^2+(S_{21})^2\big](S_{11}+S_{22})\\ &+\big[(S_{23})^2+(S_{32})^2\big](S_{22}+S_{33})\\ &+\big[(S_{13})^2+(S_{31})^2\big](S_{11}+S_{33})\}\\ &+c_{123}S_{11}S_{22}S_{33}+c_{456}\big[S_{12}S_{23}S_{31}+S_{21}S_{32}S_{13}\big].\end{aligned}$$

1.3.7. Nonlinear dynamic elasticity

1.3.7.1. *Introduction*

In recent years, the measurements of ultrasonic wave velocities as functions of stresses applied to the sample and the measurements of the amplitude of harmonics generated by the passage of an ultrasonic wave throughout the sample are in current use. These experiments and others, such as the interaction of two ultrasonic waves, are interpreted from the same theoretical basis, namely nonlinear dynamical elasticity.

A first step in the development of nonlinear dynamical elasticity is the derivation of the general equations of motion for elastic waves propagating in a solid under nonlinear elastic conditions. Then, these equations are restricted to elastic waves propagating either in an isotropic or in a cubic medium. The next step is the examination of two important cases:

(i) the generation of harmonics when *finite amplitude* ultrasonic waves travel throughout an *unstressed* medium;

(ii) the propagation of *small amplitude* ultrasonic waves when they travel throughout a *stressed* medium.

Finally, the concept of natural velocity is introduced and the experiments that can be used to determine the third- and higher-order elastic constants are described.

1.3.7.2. *Equation of motion for elastic waves*

For generality, these equations will be derived in the X configuration (initial state). It is convenient to obtain the equations of motion with the aid of Lagrange's equations. In the absence of body forces, these equations are

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial x'_i}+\frac{\partial}{\partial X_i}\frac{\partial L}{\partial\big(\partial x_i/\partial X_j\big)}=0 \qquad (1.3.7.1)$$

or

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial x'_i}+\frac{\partial}{\partial X_i}\frac{\partial L}{\partial \alpha_{ij}}=0, \qquad (1.3.7.2)$$

where L is the Lagrangian per unit initial volume and $\alpha_{ij}=\partial x_i/\partial X_j$ are the elements of the Jacobian matrix.

For adiabatic motion

$$L=\tfrac{1}{2}\rho_0 x_i'^2-\rho_0 U, \qquad (1.3.7.3)$$

where U is the internal energy per unit mass.

Combining (1.3.7.2) and (1.3.7.3), it follows that

$$\rho_0 x''^2_i=\frac{\partial}{\partial X_j}\left(\rho_0\frac{\partial U}{\partial S_{lm}}\frac{\partial S_{lm}}{\partial\alpha_{ij}}\right),$$

which can be written

$$\rho_0 x''^2_i=\frac{\partial}{\partial X_j}\left(\alpha_{il}\alpha_{jm}\rho_0\frac{\partial U}{\partial S_{lm}}\right)$$

since

$$\frac{\partial S_{lm}}{\partial\alpha_{ij}}=\tfrac{1}{2}\big(\alpha_{im}\delta_{jl}+\alpha_{il}\delta_{jm}\big).$$

Using now the equation of continuity or conservation of mass:

$$\frac{\rho_0}{\rho}=J=\det(a_{ij}),$$

and the identity of Euler, Piola and Jacobi:

$$\frac{\partial}{\partial x_j}\left(\frac{1}{J}\frac{\partial x_j}{\partial X_i}\right)=0,$$

we get an expression of Newton's law of motion:

$$\rho x''_i=\frac{\mathrm{d}T_{ij}}{\mathrm{d}X_j}\ \text{or}\ \rho u''_i=\frac{\mathrm{d}T_{ij}}{\mathrm{d}X_j} \qquad (1.3.7.4)$$

with

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

T_{ij} becomes

$$T_{ij}=\frac{1}{J}\alpha_{ik}\alpha_{jl}t_{kl}$$

since

$$t_{kl}=\rho_0\frac{\partial U}{\partial S_{kl}}.$$

t_{kl}, the thermodynamic tensor conjugate to the variable S_{kl}/ρ_0, is generally denoted as the 'second Piola–Kirchoff stress tensor'.

Using Φ, the strain energy per unit volume, Newton's law (1.3.7.4) takes the form

$$\rho x''_i=\frac{\partial}{\partial X_j}\left(\alpha_{jk}\frac{\partial\Phi}{\partial S_{ik}}\right)\quad\text{or}\quad \rho u''_i=\frac{\partial}{\partial X_j}\left(\alpha_{jk}\frac{\partial\Phi}{\partial S_{ik}}\right)$$

and

$$T_{ij}=\alpha_{jk}\frac{\partial\Phi}{\partial S_{ik}}. \qquad (1.3.7.5)$$

1.3.7.3. *Wave propagation in a nonlinear elastic medium*

As an example, let us consider the case of a plane finite amplitude wave propagating along the x_1 axis. The displacement components in this case become

$$u_1=u_1(X_1,t);\quad u_2=u_2(X_1,t);\quad u_3=u_3(X_1,t).$$

Thus, the Jacobian matrix α_{ij} reduces to

$$J=\begin{pmatrix}\alpha_{11}&0&0\\ \alpha_{21}&0&0\\ \alpha_{31}&0&0\end{pmatrix}.$$

The Lagrangian strain matrix is [equation (1.3.6.8)]

$$S=\tfrac{1}{2}\big(J^TJ-\delta\big).$$

The only nonvanishing strain components are, therefore,

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$$S_{11} = \tfrac{1}{2}\left(\alpha_{11}^2 + \alpha_{21}^2 + \alpha_{31}^2\right) - 1 = \frac{\partial u_1}{\partial X_1} + \tfrac{1}{2}\left[\left(\frac{\partial u_1}{\partial X_1}\right)^2 + \left(\frac{\partial u_2}{\partial X_1}\right)^2 + \left(\frac{\partial u_3}{\partial X_1}\right)^2\right]$$

$$S_{12} = S_{21} = \tfrac{1}{2}\frac{\partial u_2}{\partial X_1}$$

$$S_{13} = S_{31} = \tfrac{1}{2}\frac{\partial u_3}{\partial X_1}$$

and the strain invariants reduce to

$$I_1 = S_{11}; \quad I_2 = -(S_{12}S_{21} + S_{13}S_{31}); \quad I_3 = 0.$$

1.3.7.3.1. *Isotropic media*

In this case, the strain-energy density becomes

$$\Phi = \tfrac{1}{2}(\lambda + 2\mu)(S_{11})^2 + 2\mu(S_{12}S_{21} + S_{13}S_{31}) + \tfrac{1}{3}(l + 2m)(S_{11})^3 + 2mS_{11}(S_{12}S_{21} + S_{13}S_{31}). \quad (1.3.7.6)$$

Differentiating (1.3.7.6) with respect to the strains, we get

$$\frac{\partial\Phi}{\partial S_{11}} = (\lambda + 2\mu)S_{11} + (l + 2m)(S_{11})^2 + 2m(S_{12}S_{21} + S_{13}S_{31})$$

$$\frac{\partial\Phi}{\partial S_{12}} = 2\mu S_{21} + 2mS_{11}S_{21}$$

$$\frac{\partial\Phi}{\partial S_{13}} = 2\mu S_{31} + 2mS_{11}S_{31}$$

$$\frac{\partial\Phi}{\partial S_{21}} = 2\mu S_{12} + 2mS_{11}S_{12}$$

$$\frac{\partial\Phi}{\partial S_{31}} = 2\mu S_{13} + 2mS_{11}S_{13}.$$

All the other $\partial\Phi/\partial S_{ij} = 0$.

From (1.3.7.5), we derive the stress components:

$$T_{11} = \alpha_{1k}\frac{\partial\Phi}{\partial S_{1k}}; \quad T_{12} = \alpha_{2k}\frac{\partial\Phi}{\partial S_{1k}}; \quad T_{13} = \alpha_{3k}\frac{\partial\Phi}{\partial S_{1k}};$$

$$T_{21} = \alpha_{1k}\frac{\partial\Phi}{\partial S_{2k}}; \quad T_{22} = \alpha_{2k}\frac{\partial\Phi}{\partial S_{2k}}; \quad T_{23} = \alpha_{3k}\frac{\partial\Phi}{\partial S_{2k}};$$

$$T_{31} = \alpha_{1k}\frac{\partial\Phi}{\partial S_{3k}}; \quad T_{32} = \alpha_{2k}\frac{\partial\Phi}{\partial S_{3k}}; \quad T_{33} = \alpha_{3k}\frac{\partial\Phi}{\partial S_{3k}}.$$

Note that this tensor is not symmetric.

For the particular problem discussed here, the three components of the equation of motion are

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

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

$$\rho u_1'' = (\lambda + 2\mu)\frac{\partial^2 u_1}{\partial X_1^2} + [3(\lambda + 2\mu) + 2(l + 2m)]\frac{\partial u_1}{\partial X_1}\frac{\partial^2 u_1}{\partial X_1^2} + (\lambda + 2\mu + m)\left[\frac{\partial u_2}{\partial X_1}\frac{\partial^2 u_2}{\partial X_1^2} + \frac{\partial u_3}{\partial X_1}\frac{\partial^2 u_3}{\partial X_1^2}\right]$$

$$\rho u_2'' = \mu\frac{\partial^2 u_2}{\partial X_1^2} + (\lambda + 2\mu + m)\left[\frac{\partial u_1}{\partial X_1}\frac{\partial^2 u_2}{\partial X_1^2} + \frac{\partial u_2}{\partial X_1}\frac{\partial^2 u_1}{\partial X_1^2}\right]$$

$$\rho u_3'' = \mu\frac{\partial^2 u_3}{\partial X_1^2} + (\lambda + 2\mu + m)\left[\frac{\partial u_1}{\partial X_1}\frac{\partial^2 u_3}{\partial X_1^2} + \frac{\partial u_3}{\partial X_1}\frac{\partial^2 u_1}{\partial X_1^2}\right]. \quad (1.3.7.7)$$

1.3.7.3.2. *Cubic media (most symmetrical groups)*

In this case, the strain-energy density becomes

$$\Phi = \tfrac{1}{2}c_{11}(S_{11})^2 + c_{44}\left[(S_{12})^2 + (S_{21})^2 + (S_{31})^2 + (S_{13})^2\right] + c_{111}(S_{11})^3 + \tfrac{1}{2}c_{166}S_{11}\left[(S_{12})^2 + (S_{21})^2 + (S_{31})^2 + (S_{13})^2\right]. \quad (1.3.7.8)$$

Differentiating (1.3.7.8) with respect to the strain, one obtains

$$\frac{\partial\Phi}{S_{11}} = c_{11}S_{11} + 3c_{111}(S_{11})^2 + \tfrac{1}{2}c_{166}[(S_{12})^2 + (S_{21})^2 + (S_{31})^2 + (S_{13})^2)]$$

$$\frac{\partial\Phi}{S_{21}} = 2c_{44}S_{21} + c_{166}S_{11}S_{21}$$

$$\frac{\partial\Phi}{S_{31}} = 2c_{44}S_{31} + c_{166}S_{11}S_{31}.$$

All other $\partial\Phi/S_{ij} = 0$. From (1.3.7.5), we derive the stress components:

$$T_{11} = \alpha_{1k}\frac{\partial\Phi}{\partial S_{1k}}$$

$$T_{21} = \alpha_{1k}\frac{\partial\Phi}{\partial S_{2k}}$$

$$T_{31} = \alpha_{1k}\frac{\partial\Phi}{\partial S_{3k}}.$$

In this particular case, the three components of the equation of motion are

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

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

$$\rho u_1'' = c_{11}\frac{\partial^2 u_1}{\partial X_1^2} + [3c_{11} + c_{111}]\frac{\partial u_1}{\partial X_1}\frac{\partial^2 u_1}{\partial X_1^2} + (c_{11} + c_{166})\left[\frac{\partial u_2}{\partial X_1}\frac{\partial^2 u_2}{\partial X_1^2} + \frac{\partial u_3}{\partial X_1}\frac{\partial^2 u_3}{\partial X_1^2}\right]$$

$$\rho u_2'' = c_{44}\frac{\partial^2 u_2}{\partial X_1^2} + (c_{11} + c_{166})\left[\frac{\partial u_1}{\partial X_1}\frac{\partial^2 u_2}{\partial X_1^2} + \frac{\partial u_2}{\partial X_1}\frac{\partial^2 u_1}{\partial X_1^2}\right] \quad (1.3.7.9)$$

$$\rho u_3'' = c_{44}\frac{\partial^2 u_3}{\partial X_1^2} + (c_{11} + c_{166})\left[\frac{\partial u_1}{\partial X_1}\frac{\partial^2 u_3}{\partial X_1^2} + \frac{\partial u_3}{\partial X_1}\frac{\partial^2 u_1}{\partial X_1^2}\right],$$

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

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

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.

references