*International Tables for Crystallography* (2006). Vol. D, Section 1.3.7.2, pp. 94–95.



1.3.6.6. *Elastic strain-energy density*

The elastic strain-energy density has appeared in the literature in various forms. Most of the authors use the Murnaghan constants as long as isotropic solids are concerned. However, most of the literature uses Brugger's thermodynamic definition when anisotropic media are under consideration (Brugger, 1964).

The elastic strain-energy density for an isotropic medium, including third-order terms but omitting terms independent of strain, may be expressed in terms of three strain invariants, since an isotropic material is invariant with respect to rotation:

$$\Phi = \frac{\lambda + 2\mu}{2}(I_1)^2 - 2\mu I_2 + \frac{l + 2m}{3}(I_1)^3 - 2mI_1I_2 + nI_3,$$

where $\lambda$ and $\mu$ are the second-order Lamé constants, $l, m, n$ are the third-order Murnaghan constants, and $I_1, I_2, I_3$ are the three invariants of the Lagrangian strain matrix. These invariants may be written in terms of the strain components as

$$I_1 = S_{11} + S_{22} + S_{33}$$
$$I_2 = \begin{vmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{vmatrix} + \begin{vmatrix} S_{22} & S_{23} \\ S_{32} & S_{33} \end{vmatrix} + \begin{vmatrix} S_{33} & S_{31} \\ S_{13} & S_{11} \end{vmatrix}$$
$$I_3 = \begin{vmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{vmatrix}.$$

The elastic strain-energy density for an *anisotropic* medium (for example a medium belonging to the most symmetrical groups of cubic crystals) is (Green, 1973)

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

## 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

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

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

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

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 $S_{kl}/\rho_0$, is generally denoted as the 'second Piola–Kirchhoff stress tensor'.

Using $\Phi$, 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 $\alpha_{ij}$ 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)]

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

The only nonvanishing strain components are, therefore,

$$\begin{aligned} S_{11} &= \tfrac{1}{2}\left(\alpha_{11}^2 + \alpha_{21}^2 + \alpha_{31}^2\right) - 1 \\ &= \frac{\partial u_1}{\partial X_1} + \tfrac{1}{2}\left[\left(\frac{\partial u_1}{\partial X_1}\right)^2 + \left(\frac{\partial u_2}{\partial X_1}\right)^2 + \left(\frac{\partial u_3}{\partial X_1}\right)^2\right] \\ S_{12} &= S_{21} = \tfrac{1}{2}\frac{\partial u_2}{\partial X_1} \\ S_{13} &= S_{31} = \tfrac{1}{2}\frac{\partial u_3}{\partial X_1} \end{aligned}$$

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

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

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

$$\begin{aligned} \frac{\partial\Phi}{\partial S_{11}} &= (\lambda + 2\mu)S_{11} + (l + 2m)(S_{11})^2 + 2m(S_{12}S_{21} + S_{13}S_{31}) \\ \frac{\partial\Phi}{\partial S_{12}} &= 2\mu S_{21} + 2mS_{11}S_{21} \\ \frac{\partial\Phi}{\partial S_{13}} &= 2\mu S_{31} + 2mS_{11}S_{31} \\ \frac{\partial\Phi}{\partial S_{21}} &= 2\mu S_{12} + 2mS_{11}S_{12} \\ \frac{\partial\Phi}{\partial S_{31}} &= 2\mu S_{13} + 2mS_{11}S_{13}. \end{aligned}$$

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

From (1.3.7.5), we derive the stress components:

$$\begin{aligned} T_{11} &= \alpha_{1k}\frac{\partial\Phi}{\partial S_{1k}}; \quad T_{12} = \alpha_{2k}\frac{\partial\Phi}{\partial S_{1k}}; \quad T_{13} = \alpha_{3k}\frac{\partial\Phi}{\partial S_{1k}}; \\ T_{21} &= \alpha_{1k}\frac{\partial\Phi}{\partial S_{2k}}; \quad T_{22} = \alpha_{2k}\frac{\partial\Phi}{\partial S_{2k}}; \quad T_{23} = \alpha_{3k}\frac{\partial\Phi}{\partial S_{2k}}; \\ T_{31} &= \alpha_{1k}\frac{\partial\Phi}{\partial S_{3k}}; \quad T_{32} = \alpha_{2k}\frac{\partial\Phi}{\partial S_{3k}}; \quad T_{33} = \alpha_{3k}\frac{\partial\Phi}{\partial S_{3k}}. \end{aligned}$$

Note that this tensor is not symmetric.

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

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

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

$$\begin{aligned} \rho u_1'' &= (\lambda + 2\mu)\frac{\partial^2 u_1}{\partial X_1^2} + [3(\lambda + 2\mu) + 2(l + 2m)]\frac{\partial u_1}{\partial X_1}\frac{\partial^2 u_1}{\partial X_1^2} \\ &\quad + (\lambda + 2\mu + m)\left[\frac{\partial u_2}{\partial X_1}\frac{\partial^2 u_2}{\partial X_1^2} + \frac{\partial u_3}{\partial X_1}\frac{\partial^2 u_3}{\partial X_1^2}\right] \\ \rho u_2'' &= \mu\frac{\partial^2 u_2}{\partial X_1^2} + (\lambda + 2\mu + m)\left[\frac{\partial u_1}{\partial X_1}\frac{\partial^2 u_2}{\partial X_1^2} + \frac{\partial u_2}{\partial X_1}\frac{\partial^2 u_1}{\partial X_1^2}\right] \\ \rho u_3'' &= \mu\frac{\partial^2 u_3}{\partial X_1^2} + (\lambda + 2\mu + m)\left[\frac{\partial u_1}{\partial X_1}\frac{\partial^2 u_3}{\partial X_1^2} + \frac{\partial u_3}{\partial X_1}\frac{\partial^2 u_1}{\partial X_1^2}\right]. \end{aligned} \qquad (1.3.7.7)$$

1.3.7.3.2. *Cubic media (most symmetrical groups)*

In this case, the strain-energy density becomes

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

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

$$\begin{aligned} \frac{\partial\Phi}{S_{11}} &= c_{11}S_{11} + 3c_{111}(S_{11})^2 + \tfrac{1}{2}c_{166}[(S_{12})^2 + (S_{21})^2 \\ &\quad + (S_{31})^2 + (S_{13})^2)] \\ \frac{\partial\Phi}{S_{21}} &= 2c_{44}S_{21} + c_{166}S_{11}S_{21} \\ \frac{\partial\Phi}{S_{31}} &= 2c_{44}S_{31} + c_{166}S_{11}S_{31}. \end{aligned}$$

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

$$\begin{aligned} T_{11} &= \alpha_{1k}\frac{\partial\Phi}{\partial S_{1k}} \\ T_{21} &= \alpha_{1k}\frac{\partial\Phi}{\partial S_{2k}} \\ T_{31} &= \alpha_{1k}\frac{\partial\Phi}{\partial S_{3k}}. \end{aligned}$$

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



references