International Tables for Crystallography (2006). Vol. D, Section 1.3.7.3.2, pp. 95–96.

t_{kl}, the thermodynamic tensor conjugate to the variable S_{kl}/ρ_0, is generally denoted as the 'second Piola–Kirchhoff 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)]

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

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

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

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

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

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

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

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

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

references