

Thermodynamic Definition of Higher Order Elastic Coefficients

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General thermodynamic definitions of the higher order elastic coefficients of thermoelastic media are presented in tensor and engineering notation. They are natural generalizations of the customary definitions of second-order coefficients, they retain the usual conventions relating tensor and engineering stresses and strains, and they simplify thermodynamic calculations.

RECENT extension of ultrasonic techniques to high pressures and high frequencies¹⁻⁵ renewed interest in the higher order coefficients of nonlinear elasticity. We proceed to give a general definition, both in the tensor and in the abbreviated or engineering notation, of elastic coefficients of any order as partial derivatives of the thermodynamic potentials of thermoelastic media subject to finite deformation. Whereas third-order stiffnesses have already been introduced into the literature,⁶⁻⁹ the present definitions are believed to be justified since they provide the following advantages: (a) They are natural generalizations of the accepted definitions of the second-order coefficients. (b) The customary relations between tensor and abbreviated notations for stresses and strains are retained. (c) Thermodynamic relations are readily transcribed from the tensor to the abbreviated notation and vice versa. (d) No unwieldy numerical factors occur in thermodynamic calculations. (e) The coefficients defined above are identical with those encountered in anharmonic lattice theory.^{10,11}

The energy equation for conservative (nondissipative) thermoelastic media¹² gives the main thermodynamic potentials; namely, the internal energy U , the free energy F , the enthalpy H , and the Gibbs function G , in terms of the conjugate variables S and T , and t_{jk} and η_{jk}/ρ_0 , as

$$\begin{aligned} dU &= TdS + (1/\rho_0)t_{jk}d\eta_{jk} \\ dF &= -SdT + (1/\rho_0)t_{jk}d\eta_{jk} \\ dH &= TdS - (1/\rho_0)\eta_{jk}dt_{jk} \\ dG &= -SdT - (1/\rho_0)\eta_{jk}dt_{jk}, \end{aligned} \quad (1)$$

where S is the entropy, T the temperature, and the t_{jk} are the thermodynamic tensions, and the η_{jk} the Lagrangian strains.¹³ The potentials and all extensive quantities are taken per unit mass. From the relations (1) follow naturally general definitions of the elastic coefficients for any order. Namely for the adiabatic and isothermal stiffnesses c and compliances s of the n th order, for $n \geq 2$,

$$\begin{aligned} c^S_{j_1 k_1 p_1 q_1 \dots} &= \rho_0 (\partial^n U / \partial \eta_{j_1 k_1} \partial \eta_{p_1 q_1} \dots)_S \\ c^T_{j_1 k_1 p_1 q_1 \dots} &= \rho_0 (\partial^n F / \partial \eta_{j_1 k_1} \partial \eta_{p_1 q_1} \dots)_T \\ s^S_{j_1 k_1 p_1 q_1 \dots} &= -\rho_0 (\partial^n H / \partial t_{j_1 k_1} \partial t_{p_1 q_1} \dots)_S \\ s^T_{j_1 k_1 p_1 q_1 \dots} &= -\rho_0 (\partial^n G / \partial t_{j_1 k_1} \partial t_{p_1 q_1} \dots)_T. \end{aligned} \quad (2)$$

Since the strains and the thermodynamic tensions are symmetric, i.e., $\eta_{jk} = \eta_{kj}$ and $t_{jk} = t_{kj}$, only six of each set of nine variables are independent, and it is customary to introduce the Voigt¹⁴ notation: 11~1, 22~2, 33~3, 23~4, 13~5, 12~6. By convention¹⁵ we define

$$\eta_{ab} = \frac{1}{2}(1 + \delta_{ab})\eta_A \quad \text{and} \quad t_{ab} = t_A, \quad (3)$$

where lower case subscripts run from 1 to 3, and where capital subscripts run from 1 to 6. Considering the potentials now as functions of the single-subscript variables, the first of Eqs. (1) and (2) for example become

$$dU = TdS + (1/\rho_0)t_J d\eta_J \quad (1')$$

and

$$c^S_{J_1 P_1 \dots} = \rho_0 (\partial^n U / \partial \eta_{J_1} \partial \eta_{P_1} \dots)_S, \quad (2')$$

and similarly for the other three equations. Between the elastic coefficients in the tensor notation and in the abbreviated notation one has the relations

$$c_{j_1 k_1 p_1 q_1 \dots} = c_{J_1 P_1 \dots} \quad (4)$$

and

$$s_{j_1 k_1 p_1 q_1 \dots} = \frac{1}{2}(1 + \delta_{j_1 k_1}) \frac{1}{2}(1 + \delta_{p_1 q_1}) \dots s_{J_1 P_1 \dots} \quad (5)$$

From the definitions (2) and (2'), and from the symmetries of the strains and tensions follow the familiar symmetries in the subscripts of the elastic coefficients.

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⁸ R. F. S. Hearmon, *Acta Cryst.* **6**, 331 (1953).

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¹³ R. N. Thurston and K. Brugger, preceding paper, *Phys. Rev.* **133**, A1604 (1964).

¹⁴ W. Voigt, *Lehrbuch der Kristallphysik* (Teubner, Leipzig, 1928).

¹⁵ J. G. Brainerd *et al.*, *Proc. Inst. Radio Engrs.* **37**, 1378 (1949).

For example

$$c_{jkpq} \dots = c_{kjqp} \dots = c_{pqjk} \dots = \dots, \quad (6)$$

and

$$c_{JP} \dots = c_{PJ} \dots = \dots. \quad (7)$$

Two examples will illustrate the absence of unwieldy numerical factors in thermodynamic formulas and the ease with which formulas can be transcribed from the tensor to the abbreviated notation, or vice versa: A straightforward thermodynamic calculation gives the relation between the purely adiabatic third-order stiffnesses c^S_{jkpqr} defined in (2) and mixed coefficients $C_{jkpqr} = (\partial c^S_{jkpq} / \partial \eta_{rs})_T$ of the type occurring in Eq. (5.9) of the preceding paper.¹³ In the two notations they take the forms

$$c^S_{jkpqr} = C_{jkpqr} + \frac{T}{\rho_0 C_t} c^S_{rsmn} \alpha_{mn} \times \left[C_{jkpquv} \alpha_{uv} - \left(\frac{\partial c^S_{jkpq}}{\partial T} \right)_t \right] \quad (8)$$

and

$$c^S_{JPR} = C_{JPR} + \frac{T}{\rho_0 C_t} c^S_{RMA} \times \left[C_{JPV} \alpha_V - \left(\frac{\partial C^S_{JP}}{\partial T} \right)_t \right], \quad (8')$$

where C_t is the specific heat per unit mass at constant t , and the α 's are the thermal expansion coefficients

$$\alpha_{uv} = (\partial \eta_{uv} / \partial T)_t \quad \text{and} \quad \alpha_V = (\partial \eta_V / \partial T)_t. \quad (9)$$

Expanding the internal energy about the state of zero strain one obtains as the second example for $\rho_0 U(\boldsymbol{\eta}) = \rho_0 U(S, \boldsymbol{\eta}) - \rho_0 U(S, 0)$ the forms

$$\rho_0 U(\boldsymbol{\eta}) = \frac{1}{2} c^S_{jkpq} \eta_{jk} \eta_{pq} + \frac{1}{6} c^S_{jkpqr} \eta_{jk} \eta_{pq} \eta_{rs} + \dots \quad (10)$$

and

$$\rho_0 U(\boldsymbol{\eta}) = \frac{1}{2} c^S_{JP} \eta_J \eta_P + \frac{1}{6} c^S_{JPR} \eta_J \eta_P \eta_R + \dots, \quad (10')$$

where the elastic coefficients are evaluated at zero strain.

Rewriting the last equation as

$$\rho_0 U(\boldsymbol{\eta}) = \frac{1}{2} \sum_J c^S_{JJ} \eta_J^2 + \sum_{J < P} c^S_{JP} \eta_J \eta_P + \frac{1}{6} \sum_J c^S_{JJJ} \eta_J^3 + \frac{1}{2} \sum_{J \neq P} c^S_{JJP} \eta_J^2 \eta_P + \sum_{J < P < R} c^S_{JPR} \eta_J \eta_P \eta_R + \dots, \quad (11)$$

one observes that in general the numerical coefficient for any term is $1/n!$, where n is the number of equal indices of the strains. This rule allows a convenient check of energy expressions and their partial derivatives with respect to strains.

Between stiffness coefficients in the abbreviated notation introduced above and others encountered in the literature the following conversion relations hold: Murnaghan⁷:

$$c_{JP} = c_{jkpq} = \frac{1 + \delta_{jk}}{2} \frac{1 + \delta_{pq}}{2} c_{JP}^{(M)}$$

$$c_{JPR} = c_{jkpqr} = \frac{1 + \delta_{jk}}{2} \frac{1 + \delta_{pq}}{2} \frac{1 + \delta_{rs}}{2} c_{JPR}^{(M)} \quad (12)$$

Birch⁶:

$$c_{JP} = c_{JP}^{(B)}$$

$$c_{JPR} = [6/N(JPR)] c_{JPR}^{(B)}, \quad (13)$$

where $N(JPR)$ is the number of ways in which c_{JPR} can be written with tensor indices, for example $N(111) = 1$, $N(114) = 6$ and $N(456) = 48$. The third-order stiffnesses in the tensor notation are the same as those of Toupin and Bernstein,⁹ and they are six times larger than those of Hearmon.⁸

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