

1.3. ELASTIC PROPERTIES

Concerning the stress tensor, as pointed out by Thurston (1964), the stress-deformation relation is complicated in nonlinear elasticity because ‘the strain is often referred to a natural unstressed state, whereas the stress  $T_{ij}$  is defined per unit area of the deformed body’. For this reason, the differential of work done by the stress is not equal to the stress components times the differentials of the corresponding strain components. So, following Truesdell & Toupin (1960), we shall introduce a *thermodynamic tension tensor*  $t_{ij}$  defined as the first derivative of the energy with respect to strain. If the internal energy  $U$  per unit mass is considered, the *thermodynamic tension* refers to an isentropic process. Then

$$t_{ij}^\sigma = \rho_0 \left( \frac{\partial U}{\partial S_{ij}} \right)_\sigma,$$

where  $\sigma$  is the entropy and  $\rho_0$  the volumic mass in the initial state.

If the Helmholtz free energy  $F$  is considered, the thermodynamic tension refers to an isothermal process. Then

$$t_{ij}^\Theta = \rho_0 \left( \frac{\partial U}{\partial S_{ij}} \right)_\Theta,$$

where  $\Theta$  is the temperature. It will be shown in Section 1.3.7.2 that

$$T_{ij} = (1/J)\alpha_{ik}\alpha_{jl}t_{kl}.$$

1.3.6.4. Second-order and higher-order elastic stiffnesses

Following Brugger (1964), the strain-energy density, or strain energy per unit volume  $\Phi$ , is assumed to be a polynomial in the strain:

$$\Phi = \Phi_0 + c_{ij}S_{ij} + \frac{1}{2!}c_{ijkl}S_{ij}S_{kl} + \frac{1}{3!}c_{ijklmn}S_{ij}S_{kl}S_{mn}, \quad (1.3.6.9)$$

where  $\Phi = \rho_0 U(X, S_{ij})$ ,  $\Phi_0 = \rho_0 U(X, 0)$ ,  $X$  denotes the configuration of the initial state and the  $S_{ij}$ ’s are the Lagrangian finite strain-tensor components.

If the initial energy and the deformation of the body are both zero, the first two terms in (1.3.6.9) are zero. Note that  $c_{ij}$  is a stress and not an intrinsic characteristic of the material. In this expression, the elastic stiffnesses  $c_{ijkl}$  and  $c_{ijklmn}$  are the second- and third-order stiffnesses, respectively. Since the strain tensor is symmetric, pairs of subscripts can be interchanged [see equation (1.3.3.4)]:

$$\begin{aligned} c_{ijkl} &= c_{jikl} = c_{ijlk} = c_{jilk}, \\ c_{ijklmn} &= c_{jiklmn} = c_{ijlkmn} = c_{jilkmn} = c_{ijklnm} \\ &= c_{jiklnm} = c_{ijlknm} = c_{jilknm}. \end{aligned}$$

More accurately, the isentropic and the isothermal elastic stiffnesses are defined as the  $n$ th partial derivatives of the internal energy and the Helmholtz free energy, respectively. For example, the third-order isentropic and isothermal stiffnesses are, respectively,

$$\begin{aligned} c_{ijklmn}^\sigma &= \rho_0 \frac{\partial^3 U}{\partial S_{ij} \partial S_{kl} \partial S_{mn}}, \\ c_{ijklmn}^\Theta &= \rho_0 \frac{\partial^3 F}{\partial S_{ij} \partial S_{kl} \partial S_{mn}}, \end{aligned}$$

where the internal energy,  $U$ , is a function of  $X, S_{ij}$  and  $\sigma$ , and the Helmholtz free energy,  $F$ , is a function of  $X, S_{ij}$  and  $\Theta$ .

From these definitions, it follows that the Brugger stiffness coefficients depend on the initial state. *When no additional information is given, the initial state is the natural state.*

Table 1.3.6.1. Number of independent third-order elastic stiffnesses for each Laue class

Laue class	Number of independent components
$\bar{1}, 1$	56
$2/m, 2, m$	32
$mmm, 222, 2mm$	20
$\bar{3}, 3$	20
$\bar{3}, 32, 3m$	14
$4/m, 4, \bar{4}$	16
$4/mmm, 422, \bar{4}2m, 42m$	12
$6/m, 6, \bar{6}$	12
$6/mmm, 622, \bar{6}2m, 62m$	10
$m\bar{3}, 23$	8
$m\bar{3}m, 432, \bar{4}32$	6
$\infty(A_\infty/M)C, \infty A_\infty$	3

The third-order stiffnesses form a sixth-rank tensor containing  $3^6 = 729$  components, of which 56 are independent for a triclinic crystal and 3 for isotropic materials. The independent components of a sixth-rank tensor can be obtained for any point group using the accompanying software to this volume. They are listed in Table 1.3.6.1 for each Laue class. They can be reduced to three-index coefficients. Table 1.3.6.2 gives the values of the third-order stiffnesses of some materials.

The three independent constants for isotropic materials are often taken as  $c_{123}$ ,  $c_{144}$  and  $c_{456}$  and denoted respectively by  $\nu_1, \nu_2, \nu_3$ , the ‘third-order Lamé constants’.

The ‘third-order Murnaghan constants’ (Murnaghan, 1951), denoted by  $l, m, n$ , are given in terms of the Brugger constants by the relations

$$l = \frac{1}{2}c_{112}; \quad m = c_{155}; \quad n = 4c_{456}.$$

Similarly, the fourth-order stiffnesses form an eighth-rank tensor containing  $3^8 = 6561$  components, 126 of which are independent for a triclinic crystal and 11 for isotropic materials (the independent components of a sixth-rank tensor can be obtained for any point group using the accompanying software to this volume).

For a solid under finite strain conditions, the definition of the elastic compliance tensor has to be reconsidered. In linear elasticity, the second-order elastic compliances  $s_{ijkl}$  were defined through the relations (1.3.3.2):

$$S_{ij} = s_{ijkl}T_{kl} \quad \text{or} \quad s_{ijkl} = \frac{\partial S_{ij}}{\partial T_{kl}},$$

while, in nonlinear elasticity, one has

$$s_{ijkl} = \frac{\partial S_{ij}}{\partial t_{kl}},$$

where

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

1.3.6.5. Expansion of elastic constants for small initial stress

In most experiments, the initial stress is small compared with the second-order elastic constants (for example, 1 GPa hydrostatic pressure compared with the usual value  $c_{ijkl} = 100$  GPa). Consequently, the deformation between the initial (stressed) state and the natural (unstressed) state is small compared with 1. For this reason, it is convenient to expand the elastic constants in the initial state as a power series in the strain about the natural state. *To avoid confusion, we introduce new notations:  $\bar{X}$  now represents the coordinates in the natural or unstressed state;  $X$  represents the coordinates in the initial or homogeneously*

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Table 1.3.6.2. Third-order elastic stiffnesses of some materials in (GPa)<sup>-1</sup> (after Every & McCurdy, 1992)

(a) Trigonal.

Material	c <sub>111</sub>	c <sub>112</sub>	c <sub>113</sub>	c <sub>114</sub>	c <sub>123</sub>	c <sub>124</sub>	c <sub>133</sub>	c <sub>134</sub>	c <sub>144</sub>	c <sub>155</sub>	c <sub>222</sub>	c <sub>333</sub>	c <sub>344</sub>	c <sub>444</sub>
Al <sub>2</sub> O <sub>3</sub>	-3870	-1090	-963	55	-289	-39	-922	-131	-302	-1160	-4520	-3340	-1090	-19
CaCO <sub>3</sub>	-579	-147	-193	218	-41	10	-239	82	-69	-139	-675	-498	-195	33

(b) Tetragonal.

Material	c <sub>111</sub>	c <sub>112</sub>	c <sub>113</sub>	c <sub>123</sub>	c <sub>133</sub>	c <sub>144</sub>	c <sub>155</sub>	c <sub>166</sub>	c <sub>333</sub>	c <sub>344</sub>	c <sub>366</sub>	c <sub>456</sub>
KH <sub>2</sub> PO <sub>4</sub>	-538	-291	-259	-258	67	-8	-35	-30	-912	-27	-19	8
TeO <sub>2</sub>	-160	-600	-140	-110	180	-41	36	-640	-2110	-54	-260	-250

(c) Hexagonal.

Material	c <sub>111</sub>	c <sub>112</sub>	c <sub>113</sub>	c <sub>123</sub>	c <sub>133</sub>	c <sub>144</sub>	c <sub>155</sub>	c <sub>222</sub>	c <sub>333</sub>	c <sub>344</sub>
Cd	-2060	-114	-197	-110	-268	227	-332	-2020	-516	-171
CdS	-459	-207	-182	-235	-306	-27	9	-355	-327	-69
Co	-6710	-1454	-766	-429	-511	133	-1486	-5788	-6347	-210
Mg	-663	-178	30	-76	-86	-30	-58	-864	-726	-193
Zn	-1760	-440	-270	-210	-350	-10	250	-2410	-720	-440

(d) Cubic.

Material	c <sub>111</sub>	c <sub>112</sub>	c <sub>123</sub>	c <sub>144</sub>	c <sub>155</sub>	c <sub>456</sub>
LiF	-1920	-330	-40	100	-325	43
MgO	-4900	-95	-69	113	-659	147
KBr	-532	-49	69	22	-28	-35
KCl	-610	-31	9	19	-35	17
NaCl	-866	-37	38	25	-78	18
Diamond	-6260	-2260	112	-674	-2860	-823
GaAs	-620	-392	-62	8	-274	-43
Ge	-714	-388	-34	-9	-303	-48
Si	-795	-445	-75	15	-310	-86
ZnSe	-827	-136	-511	222	-265	-278
Al	-1224	-373	25	-64	-368	-27
Cu	-1271	-814	-50	-3	-780	-95
Au	-1730	-922	-233	-13	-648	-12
Fe	-2705	-626	-575	-836	-531	-721
Ni	-2104	-1345	59	-180	-757	-42

strained state;  $u_i = x_i - X_i$  are the components of displacement. All letters with superscript bar refer to the natural state; for example,  $\bar{S}_{ij}$  denotes the Lagrangian strain in the natural state;  $\bar{U} = \bar{U}(\bar{X}, \bar{S}_{ij})$ .

Now, in order to relate the properties at  $X$  to those at  $\bar{X}$ , we need to specify the strain from  $\bar{X}$  to  $X$ . Let

$$a_{ij} = \frac{\partial X_i}{\partial \bar{X}_j} = \bar{\alpha}_{ij}.$$

Consequently,

$$\frac{\partial \bar{S}_{ij}}{\partial S_{mn}} = a_{mi} a_{nj}.$$

The second-order elastic constants at  $X$  can be expressed in terms of the second- and third-order elastic constants at  $\bar{X}$ :

$$c_{ijkl} = \rho_0 \frac{\partial^2 U}{\partial S_{ij} \partial S_{kl}} = \rho_0 \frac{\partial^2 \bar{U}}{\partial \bar{S}_{mn} \partial \bar{S}_{pq}} a_{im} a_{jn} a_{kp} a_{lq}$$

or

$$c_{ijkl} = \frac{\rho_0}{\rho_0} \left( \bar{c}_{mnpq} + \bar{c}_{mnpqrs} S_{rs} + \frac{1}{2!} \bar{c}_{mnpqrstuv} S_{rs} S_{tu} + \dots \right) a_{im} a_{jn} a_{kp} a_{lq}.$$

This expression holds for both isentropic and isothermal elastic constants.

## 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:

$$\Phi = \frac{\lambda + 2\mu}{2} (I_1)^2 - 2\mu I_2 + \frac{l + 2m}{3} (I_1)^3 - 2m I_1 I_2 + n I_3,$$

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

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

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)