Table 1.3.6.2. *Third-order elastic stiffnesses of some materials in (GPa)$^{-1}$ (after Every & McCurdy, 1992)*

(*a*) Trigonal.

Material	c_{111}	c_{112}	c_{113}	c_{114}	c_{123}	c_{124}	c_{133}	c_{134}	c_{144}	c_{155}	c_{222}	c_{333}	c_{344}	c_{444}
Al_2O_3	−3870	−1090	−963	55	−289	−39	−922	−131	−302	−1160	−4520	−3340	−1090	−19
$CaCO_3$	−579	−147	−193	218	−41	10	−239	82	−69	−139	−675	−498	−195	33

(*b*) Tetragonal.

Material	c_{111}	c_{112}	c_{113}	c_{123}	c_{133}	c_{144}	c_{155}	c_{166}	c_{333}	c_{344}	c_{366}	c_{456}
KH_2PO_4	−538	−291	−259	−258	67	−8	−35	−30	−912	−27	−19	8
TeO_2	−160	−600	−140	−110	180	−41	36	−640	−2110	−54	−260	−250

(*c*) Hexagonal.

Material	c_{111}	c_{112}	c_{113}	c_{123}	c_{133}	c_{144}	c_{155}	c_{222}	c_{333}	c_{344}
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_{111}	c_{112}	c_{123}	c_{144}	c_{155}	c_{456}
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; $\bar{U} = U(\bar{X}, \bar{S}_{ij})$.

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

$$c_{ijkl} = \frac{\rho_0}{\bar{\rho}_0}\left(\bar{c}_{mnpq} + \bar{c}_{mnpqrs}S_{rs} + \frac{1}{2!}\bar{c}_{mnpqrstu}S_{rs}S_{tu} + \right)a_{im}a_{jn}a_{kp}a_{lq}.$$

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:

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

where λ and μ 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)