

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

$$\left. \begin{array}{l} i = j; \quad k = l \\ i = j; \quad k \neq l \\ i \neq j; \quad k = l \\ i \neq j; \quad k \neq l \end{array} \right\} \begin{array}{l} \text{compliances} \\ s_{\alpha\beta} = s_{iill} \\ s_{\alpha\beta} = s_{iill} + s_{iilk} \\ s_{\alpha\beta} = s_{ijll} + s_{jill} \\ s_{\alpha\beta} = s_{ijkl} + s_{jikl} + s_{ijlk} + s_{jilk} \end{array} \left. \begin{array}{l} \text{stiffnesses} \\ c_{\alpha\beta} = cijkl. \end{array} \right\} \quad (1.3.3.6)$$

Using these notations and Voigt's notations for the strain and stress tensors, equations (1.3.3.2) become:

$$\begin{aligned} S_{\alpha\beta} &= s_{\alpha\beta} T_{\beta} \\ T_{\alpha\beta} &= c_{\alpha\beta} S_{\beta}. \end{aligned} \quad (1.3.3.7)$$

For instance, the first of these two relations is written, once developed, as

$$\begin{pmatrix} S_1 \\ S_2 \\ S_3 \\ S_4 \\ S_5 \\ S_6 \end{pmatrix} = \begin{pmatrix} s_{11} & s_{12} & s_{13} & s_{14} & s_{15} & s_{16} \\ s_{12} & s_{22} & s_{23} & s_{24} & s_{25} & s_{26} \\ s_{13} & s_{23} & s_{33} & s_{34} & s_{35} & s_{36} \\ s_{14} & s_{24} & s_{34} & s_{44} & s_{45} & s_{46} \\ s_{15} & s_{25} & s_{35} & s_{45} & s_{55} & s_{56} \\ s_{16} & s_{26} & s_{36} & s_{46} & s_{56} & s_{66} \end{pmatrix} \begin{pmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{pmatrix}. \quad (1.3.3.8)$$

Matrices $s_{\alpha\beta}$ and $c_{\alpha\beta}$ are the inverse of each other. It is important to note that they are matrices and not tensors. One cannot apply to them the usual rules of transformation under a change of base since they are only valid for the components of a tensor. In cases where the coordinate system is changed, it is necessary to use the components s_{ijkl} and c_{ijkl} or to establish the rules of transformation for $s_{\alpha\beta}$ and $c_{\alpha\beta}$.

(iii) *Symmetry of the crystal*: the reduction of the number of independent components of the matrices $s_{\alpha\beta}$ and $c_{\alpha\beta}$ was discussed in Section 1.1.4.10.6. As a summary, Table 1.3.3.1 gives the number of independent components for each Laue class.

(iv) *Cauchy relation*: the form that the strain energy of a discrete-particle structure takes when its potential energy depends only on the magnitude of the distance separating pairs of particles is called the central or point-to-point force law. It is shown that, when the cohesive forces have this special form, structures that are such that every atom is situated at a centre of symmetry have elastic constants that are totally symmetric in their four indices. Thus

$$c_{ijkl} = c_{ikjl} = c_{ijlk}$$

in addition to the symmetries required by the previous considerations. This additional symmetry implies the following relations between the two-index components:

$$\begin{aligned} c_{23} &= c_{44}; & c_{14} &= c_{56} \\ c_{13} &= c_{55}; & c_{25} &= c_{46} \\ c_{12} &= c_{66}; & c_{36} &= c_{45}. \end{aligned}$$

Table 1.3.3.1. Number of independent components of the elastic compliances and stiffnesses for each Laue class

Laue class	No. of independent components
$\bar{1}, 1$	21
$2/m, 2, m$	13
$mmm, 222, 2mm$	9
$\bar{3}, 3$	7
$\bar{3}m, 32, 3m$	6
$4/m, 4, 4$	7
$4/mmm, 422, 42m, 42m$	6
$6/m, 6, 6$	5
$6/mmm, 622, 62m, 62m$	5
$m\bar{3}, 23$	3
$m\bar{3}m, 432, \bar{4}32$	3
$\infty A_{\infty}/MC, \infty A_{\infty}$	2

These are known as the Cauchy relations. The further symmetry implied by the Cauchy relations reduces the maximum number of independent constants from 21 to 15. In crystal structures for which they might be valid, the extent to which these relations are fulfilled is often used to assess the validity of the assumption of a central-force law. It is important to apply such a test only to structures having the necessary symmetry properties for Cauchy relations to hold. For instance, f.c.c and b.c.c. metals have the required symmetry (an inversion centre at each atomic site), while diamond, silicon and germanium do not. Consequently, any apparent fulfilment of the Cauchy relation $c_{12} = c_{66}$ for a diamond-type structure offers no ground for conclusions about the nature of the force field.

1.3.3.2.3. Passage from elastic compliances $s_{\alpha\beta}$ to elastic stiffnesses $c_{\alpha\beta}$

We have noted already that the matrix $c_{\alpha\beta}$ is the inverse of the matrix $s_{\alpha\beta}$. These matrices can be written for cubic and isotropic materials as follows:

$$\begin{aligned} s_{\alpha\beta} &= \begin{pmatrix} s_{11} & s_{12} & s_{12} & 0 & 0 & 0 \\ s_{12} & s_{11} & s_{12} & 0 & 0 & 0 \\ s_{12} & s_{12} & s_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & s_{44} \end{pmatrix} \\ c_{\alpha\beta} &= \begin{pmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{pmatrix}, \end{aligned}$$

where we have, for isotropic materials,

$$\begin{aligned} s_{44} &= 2(s_{11} - s_{12}) \\ c_{44} &= \frac{1}{2}(c_{11} - c_{12}). \end{aligned} \quad (1.3.3.9)$$

We easily find that

$$\begin{aligned} s_{11} &= \frac{c_{11} + c_{12}}{(c_{11} - c_{12})(c_{11} + 2c_{12})}; & c_{11} &= \frac{s_{11} + s_{12}}{(s_{11} - s_{12})(s_{11} + 2s_{12})}; \\ s_{12} &= \frac{-c_{12}}{(c_{11} - c_{12})(c_{11} + 2c_{12})}; & c_{12} &= \frac{-s_{12}}{(s_{11} - s_{12})(s_{11} + 2s_{12})}; \\ s_{44} &= \frac{1}{c_{44}}; & c_{44} &= \frac{1}{s_{44}}. \end{aligned}$$

The coefficient c_{44} is sometimes called the *rigidity modulus*.

1.3.3.3. Elastic strain energy

Expression (1.3.2.7) of the strain energy stored per unit volume in a medium for a small deformation can be integrated when the medium is strained under a stress T_{ij} according to linear elasticity. Applying relation (1.3.3.2), one gets for the density of strain energy

$$W = \frac{1}{2} T_{ij} S_{ij} = \frac{1}{2} c_{ijkl} S_{ij} S_{kl}. \quad (1.3.3.10)$$

1.3.3.4. Particular elastic constants

1.3.3.4.1. Volume compressibility

Let us apply a hydrostatic pressure (Section 1.3.2.5.2). The medium undergoes a relative variation of volume $\Delta V/V = S_1 + S_2 + S_3$ (the cubic dilatation, Section 1.3.1.3.2). If one

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replaces in (1.3.3.8) the stress distribution by a hydrostatic pressure, one obtains for the components of the strain tensor

$$\begin{aligned} S_1 &= -p(s_{11} + s_{12} + s_{13}) \\ S_2 &= -p(s_{12} + s_{22} + s_{23}) \\ S_3 &= -p(s_{13} + s_{23} + s_{33}). \end{aligned}$$

From this, we deduce the volume compressibility, χ , which is the inverse of the *bulk modulus*, κ :

$$\chi = \kappa^{-1} = -\frac{1}{p} \frac{\delta V}{V} = s_{11} + s_{22} + s_{33} + 2(s_{12} + s_{23} + s_{13}). \quad (1.3.3.11)$$

This expression reduces for a cubic or isotropic medium to

$$\chi = \kappa^{-1} = 3(s_{11} + 2s_{12}). \quad (1.3.3.12)$$

1.3.3.4.2. Linear compressibility

Under the action of a hydrostatic pressure, each vector assumes a different elongation. This elongation is given by equation (1.3.1.6):

$$\frac{u_r}{r} = \frac{S_{ij}x_i x_j}{r^2} = S_{ij}\alpha_i \alpha_j = s_{ijkl} T_{kl} \alpha_i \alpha_j,$$

where the α_i 's are the direction cosines of \mathbf{r} . The coefficient of linear compressibility is, by definition, $(-1/p)(u_r/r)$. Replacing T_{kl} by its value $-p\delta_{kl}$, we obtain for the coefficient of linear compressibility

$$-\frac{1}{p} \frac{u_r}{r} = s_{ijkl} \alpha_i \alpha_j.$$

In the case of a cubic or isotropic medium, this expression reduces to

$$-\frac{1}{p} \frac{u_r}{r} = s_{11} + 2s_{12}.$$

The coefficient of linear compressibility is then equal to one third of the coefficient of volume compressibility. We note that the quadric of elongations is a sphere.

1.3.3.4.3. Young's modulus, Poisson's ratio

If the applied stress reduces to a uniaxial stress, $T_{11} = T$, the strain tensor is of the form

$$S_\alpha = s_{1\alpha} T.$$

In particular,

$$S_1 = s_{11} T; \quad S_2 = s_{12} T.$$

We deduce from this that Young's modulus (equation 1.3.3.1) is

$$E = 1/s_{11}. \quad (1.3.3.13)$$

The elongation of a bar under the action of a uniaxial stress is characterized by S_1 and the diminution of the cross section is characterized by S_2 and S_3 . For a cubic material, the relative diminution of the diameter is

$$S_2 = S_3 = s_{12} T.$$

One deduces from this that s_{12} is necessarily of opposite sign to s_{11} and one calls the ratio $\nu = -s_{12}/s_{11}$ *Poisson's ratio*.

Putting this value into expression (1.3.3.12) for the coefficient of compressibility in cubic or isotropic materials gives

$$\kappa^{-1} = 3s_{11}(1 - 2\nu). \quad (1.3.3.14)$$

As the coefficient of compressibility, by definition, is always positive, we have

$$0 < \nu < 0.5.$$

In practice, Poisson's ratio is always close to 0.3. It is a dimensionless number. The quantity $s_{44}/2(s_{11} - s_{12})$ represents the departure from isotropy of the material and is the anisotropy factor. It is to be noted that cubic materials are not isotropic for elastic properties. Table 1.3.3.2 gives the values of s_{11} , s_{12} , s_{44} , ν and $s_{44}/2(s_{11} - s_{12})$ for a few cubic materials.

1.3.3.4.4. Variation of Young's modulus with orientation

It is interesting to calculate Young's modulus in any direction. For this it is sufficient to change the axes of the tensor s_{ijkl} . If A is the matrix associated with the change of axes, leading to the direction x_1 changing to the direction x'_1 , then Young's modulus in this new direction is

$$E' = 1/s'_{11}$$

with

$$s'_{11} = s'_{1111} = A_{1i} A_{1j} A_{1k} A_{1l} s_{ijkl}. \quad (1.3.3.15)$$

Table 1.3.3.2. Elastic compliances of some cubic materials in (GPa)⁻¹ (after Landoldt-Börnstein, 1979)

Material	s_{11}	s_{12}	s_{44}	ν	$s_{44}/2(s_{11} - s_{12})$
Ag	22.9	-9.8	22.1	0.428	0.338
Al	16.0	-5.8	35.3	0.362	0.810
C (diamond)	1.12	-0.14	1.83	0.125	0.726
Cu	15.0	-6.3	13.3	0.42	0.312
Fe	7.67	-2.83	8.57	0.369	0.408
Ge	9.73	-2.64	14.9	0.271	0.602
Mo	2.71	-0.74	9.00	0.273	1.304
Ni	7.67	-2.93	8.23	0.382	0.388
Pb	93.7	-43.04	68.0	0.459	0.249
Si	7.74	-2.16	12.60	0.279	0.636
W	2.49	-0.70	6.35	0.281	0.995
LiF	11.6	-3.35	15.8	0.289	0.528
MgO	4.01	-0.96	6.47	0.239	0.651
NaCl	23.9	-3.20	78.7	0.133	1.452
GaAs	11.75	-3.66	16.8	0.311	0.545
ZnS	19.7	-7.6	22.6	0.386	0.414
BaTiO ₃	8.33	-2.68	9.24	0.322	0.420
Adamantane	240	-79	295	0.329	0.462
Almandine (Fe ₃ Al ₂ Si ₃ O ₁₂)	4.036	-1.093	10.77	0.271	1.050
Spinel (MgAl ₂ O ₄)	5.80	-2.05	6.49	0.353	0.413

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The matrix coefficients A_{li} are the direction cosines of Ox'_1 with respect to the axes Ox_1 , Ox_2 and Ox_3 . In spherical coordinates, they are given by (Fig. 1.3.3.3)

$$A_{11} = \cos \theta \sin \varphi, \quad A_{12} = \sin \theta \sin \varphi, \quad A_{13} = \cos \varphi,$$

where θ is the angle between Ox'_1 and Ox_1 , and φ is the angle between Ox'_1 and Ox_3 . Using the reduction of s_{ijkl} for the various crystal classes (Section 1.1.4.9.9), we find, in terms of the reduced two-index components, the following.

(i) *Triclinic system* (groups 1, $\bar{1}$):

$$\begin{aligned} s'_{11} = & [s_{11} \cos^4 \theta + s_{22} \sin^4 \theta + (2s_{12} + s_{66}) \sin^2 2\theta/4 \\ & + (s_{16} \cos \theta + s_{26} \sin \theta) \sin 2\theta] \sin^4 \varphi \\ & + 2\{[(s_{25} + s_{46}) \sin \theta + (s_{14} + s_{56}) \cos \theta] \sin 2\theta/2 \\ & + s_{15} \cos^3 \theta + s_{24} \sin^3 \theta\} \cos \varphi \sin^3 \varphi \\ & + [(2s_{23} + s_{44}) \sin^2 \theta + (2s_{13} + s_{55}) \cos^2 \theta \\ & + (s_{36} + s_{45}) \sin 2\theta] \sin^2 2\varphi/4 \\ & + 2(s_{35} \cos \theta + s_{34} \sin \theta) \cos^3 \varphi \sin \varphi + s_{33} \cos^4 \varphi. \end{aligned}$$

(ii) *Monoclinic system* (groups 2, m , $2/m$):

$$\begin{aligned} s'_{11} = & [s_{11} \cos^4 \theta + s_{22} \sin^4 \theta + (2s_{12} + s_{66}) \sin^2 2\theta/4] \sin^4 \varphi \\ & + 2[(s_{25} + s_{46}) \sin^2 \theta + s_{15} \cos^2 \theta] \cos \varphi \sin^3 \varphi \cos \theta \\ & + [(2s_{23} + s_{44}) \sin^2 \theta + (2s_{13} + s_{55}) \cos^2 \theta] \sin^2 2\varphi/4 \\ & + 2s_{35} \cos^3 \varphi \sin \varphi \cos \theta + s_{33} \cos^4 \varphi. \end{aligned}$$

(iii) *Orthorhombic system* (groups 222, $2mm$, mmm):

$$\begin{aligned} s'_{11} = & [s_{11} \cos^4 \theta + s_{22} \sin^4 \theta + (2s_{12} + s_{66}) \sin^2 2\theta/4] \sin^4 \varphi \\ & + [(2s_{23} + s_{44}) \sin^2 \theta + (2s_{13} + s_{55}) \cos^2 \theta] \sin^2 2\varphi/4 \\ & + s_{33} \cos^4 \varphi. \end{aligned}$$

(iv) *Trigonal system* (groups 3, $\bar{3}$):

$$\begin{aligned} s'_{11} = & s_{11} \sin^4 \varphi + s_{33} \cos^4 \varphi + (2s_{13} + s_{44}) \sin^2 2\varphi/4 \\ & + (s_{14} \sin 3\theta - s_{25} \cos 3\theta) \sin 2\varphi \sin^2 \varphi. \end{aligned}$$

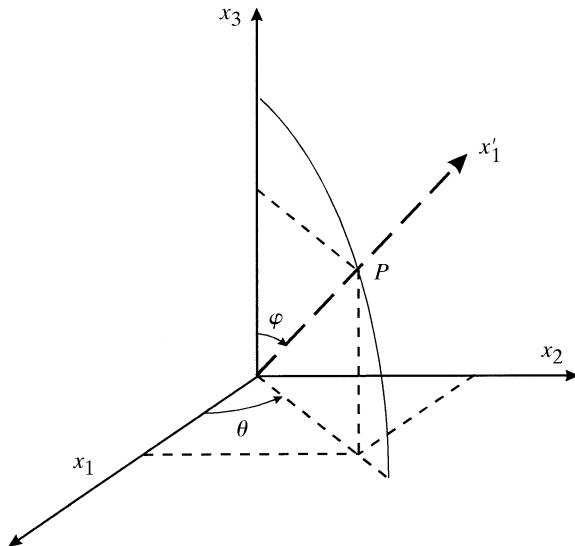


Fig. 1.3.3.3. Spherical coordinates.

(v) *Trigonal system* (groups 32, $3m$, $\bar{3}m$):

$$\begin{aligned} s'_{11} = & s_{11} \sin^4 \varphi + s_{33} \cos^4 \varphi + (2s_{13} + s_{44}) \sin^2 2\varphi/4 \\ & + s_{14} \sin 3\theta \sin 2\varphi \sin^2 \varphi. \end{aligned}$$

(vi) *Tetragonal system* (groups 4, $\bar{4}$, $4/m$):

$$\begin{aligned} s'_{11} = & \{s_{11} + [s_{66} - 2(s_{11} - s_{12})] \sin^2 2\theta/4\} \sin^4 \varphi + s_{33} \cos^4 \varphi \\ & + (2s_{13} + s_{44}) \sin^2 2\varphi/4 + s_{16} \sin 4\theta \sin^4 \varphi/2. \end{aligned}$$

(vii) *Tetragonal system* (groups 422, $\bar{4}2m$, $4mm$, $4/mmm$):

$$\begin{aligned} s'_{11} = & \{s_{11} + [s_{66} - 2(s_{11} - s_{12})] \sin^2 2\theta/4\} \sin^4 \varphi + s_{33} \cos^4 \varphi \\ & + (2s_{13} + s_{44}) \sin^2 2\varphi/4. \end{aligned}$$

(viii) *Hexagonal system*:

$$s'_{11} = s_{11} \sin^4 \varphi + s_{33} \cos^4 \varphi + (2s_{13} + s_{44}) \sin^2 2\varphi/4.$$

(ix) *Cubic system*:

$$s'_{11} = s_{11} + [s_{44} - 2(s_{11} - s_{12})] \sin^2 \varphi [\cos^2 \varphi + \sin^2 2\theta \sin^2 \varphi/4].$$

This expression reduces to s_{11} if $s_{44} - 2(s_{11} - s_{12}) = 0$ and we retrieve the relation between elastic compliances in an isotropic material (Sections 1.1.4.10.4 and 1.3.3.2.3).

The representation surface of s_{11} , the inverse of Young's modulus, is illustrated in Figure 1.3.3.4 for crystals of different symmetries. As predicted by the Neumann principle, the representation surface is invariant with respect to the symmetry elements of the point group of the crystal but, as stated by the Curie laws, its symmetry can be larger. In the examples of Fig. 1.3.3.4, the symmetry of the surface is the same as that of the point group for sodium chloride (Fig. 1.3.3.4a), tungsten (Fig. 1.3.3.4b) and aluminium (Fig. 1.3.3.4c), which have $m\bar{3}m$ as point group, for tin (Fig. 1.3.3.4e, $4/mmm$) and for calcite (Fig. 1.3.3.4f, $\bar{3}m$). But in the case of zinc (Fig. 1.3.3.4d, $6/mmm$), the surface is of revolution and has a larger symmetry. It is interesting to compare the differences in shapes of the representation surfaces for the three cubic crystals, depending on the value of the anisotropy factor, which is larger than 1 for sodium chloride, smaller than 1 for aluminium and close to 1 for tungsten (see Table 1.3.3.2). In this latter case, the crystal is pseudo-isotropic and the surface is practically a sphere.

1.3.3.5. Isotropic materials

The isotropy relation between elastic compliances and elastic stiffnesses is given in Section 1.3.3.2.3. For reasons of symmetry, the directions of the eigenvectors of the stress and strain tensors are necessarily the same in an isotropic medium. If we take these directions as axes, the two tensors are automatically diagonalized and the second relation (1.3.3.7) becomes

$$\begin{aligned} T_1 &= c_{11}S_1 + c_{12}(S_2 + S_3) \\ T_2 &= c_{12}S_1 + c_{11}S_2 + c_{12}S_3 \\ T_3 &= c_{12}(S_1 + S_2) + c_{11}S_3. \end{aligned}$$

These relations can equally well be written in the symmetrical form

$$\begin{aligned} T_1 &= (c_{11} - c_{12})S_1 + c_{12}(S_1 + S_2 + S_3) \\ T_2 &= (c_{11} - c_{12})S_2 + c_{12}(S_1 + S_2 + S_3) \\ T_3 &= (c_{11} - c_{12})S_3 + c_{12}(S_1 + S_2 + S_3). \end{aligned}$$