

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

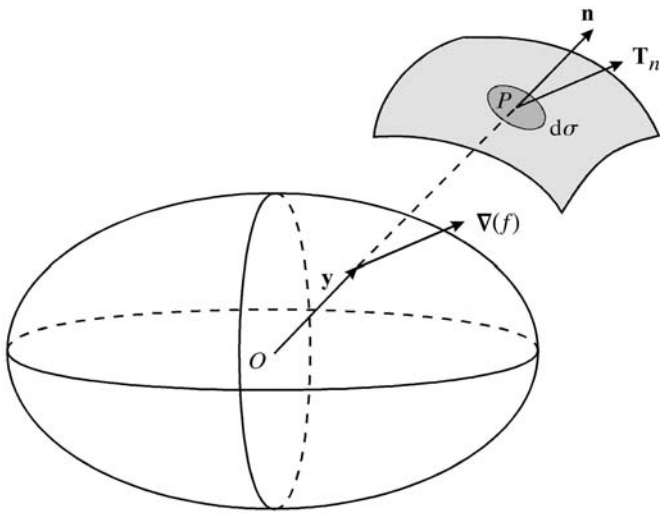


Fig. 1.3.2.7. The stress quadric: application to the determination of the stress applied to a surface element. The surface of the medium is shaded in light grey and a small surface element,  $d\sigma$ , is shaded in medium grey. The stress at  $P$  is proportional to  $\nabla(f)$  at the intersection of  $OP$  with the stress quadric.

$$\delta x'_i - \delta \Delta x_i = \delta S_{ij} \delta x_j.$$

We shall take as the position of  $Q$  the point of application of the forces at face 1, *i.e.* its centre with coordinates  $\Delta x_1, 0, 0$  (Fig. 1.3.2.8). The area of face 1 is  $4\Delta x_2 \Delta x_3$  and the forces arising from the stresses  $T_{11}$  and  $T_{12}$  are equal to  $4\Delta x_2 \Delta x_3 T_{11}$  and  $4\Delta x_2 \Delta x_3 T_{12}$ , respectively. The relative displacement of  $Q$  parallel to the line of action of  $T_{11}$  is  $\Delta x_1 \delta S_{11}$  and the corresponding displacement along the line of action of  $T_{12}$  is  $\Delta x_1 \delta S_{21}$ . The work of the corresponding forces is therefore

$$\begin{aligned} \text{for } T_{11} : & 4\Delta x_1 \Delta x_2 \Delta x_3 T_{11} \delta S_{11} \\ \text{for } T_{12} : & 4\Delta x_1 \Delta x_2 \Delta x_3 T_{12} \delta S_{21}. \end{aligned}$$

The work of the forces applied to the face 1' is the same ( $T_{11}$ ,  $T_{12}$  and  $x_1$  change sign simultaneously). The works corresponding to the faces 1 and 1' are thus  $T_{11} \delta S_{11} \Delta \tau$  and  $T_{12} \delta S_{21} \Delta \tau$  for the two stresses, respectively. One finds an analogous result for each of the other components of the stress tensor and the total work per unit volume is

$$\delta W = T_{ij} \delta S_{ji}. \tag{1.3.2.7}$$

1.3.3. Linear elasticity

1.3.3.1. Hooke's law

Let us consider a metallic bar of length  $l_o$  loaded in pure tension (Fig. 1.3.3.1). Under the action of the uniaxial stress  $T = F/A$  ( $F$  applied force,  $A$  area of the section of the bar), the bar elongates and its length becomes  $l = l_o + \Delta l$ . Fig. 1.3.3.2 relates the variations of  $\Delta l$  and of the applied stress  $T$ . The curve representing the traction is very schematic and does not correspond to any real case. The following result, however, is common to all concrete situations:

(i) If  $0 < T < T_o$ , the deformation curve is reversible, *i.e.* if one releases the applied stress the bar resumes its original form. To a first approximation, the curve is linear, so that one can write *Hooke's law*:

$$\frac{\Delta l}{l} = \frac{1}{E} T, \tag{1.3.3.1}$$

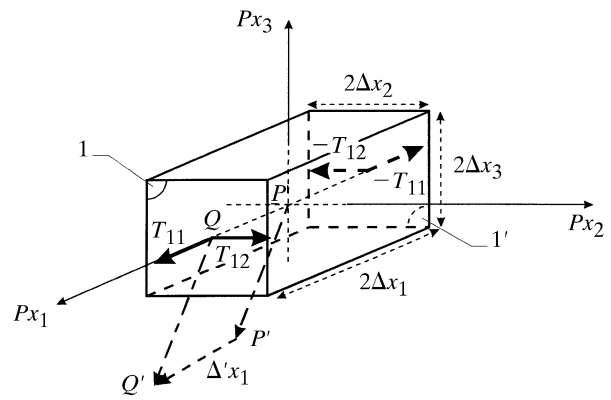


Fig. 1.3.2.8. Determination of the energy density in a deformed medium.  $PP'$  represents the displacement of the small parallelepiped during the deformation. The thick arrows represent the forces applied to the faces 1 and 1'.

where  $E$  is the elastic stiffness, also called Young's modulus. The physical mechanism at the origin of elasticity is the deformation of the chemical bonds between atoms, ions or molecules in the solid, which act as so many small springs. The reaction of these springs to an applied stress is actually anharmonic and Hooke's law is only an approximation: a Taylor expansion up to the first term. A rigorous treatment of elasticity requires nonlinear phenomena to be taken into account. This is done in Section 1.3.6. The stress below which the strain is recoverable when the stress is removed,  $T_o$ , is called the *elastic limit*.

(ii) If  $T > T_o$ , the deformation curve is no longer reversible. If one releases the applied stress, the bar assumes a permanent deformation. One says that it has undergone a *plastic* deformation. The region of the deformation is ultimately limited by rupture (symbolized by an asterisk on Fig. 1.3.3.2). The plastic deformation is due to the formation and to the movement of lattice defects such as dislocations. The material in its initial state, before the application of a stress, is not free in general from defects and it possesses a complicated history of deformations. The proportionality constant between stresses and deformations in the elastic region depends on the interatomic force constants and is an intrinsic property, very little affected by the presence of defects. By contrast, the limit,  $T_o$ , of the elastic region depends to a large extent on the defects in the material and on its history. It is

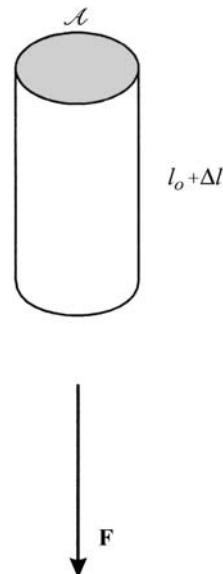


Fig. 1.3.3.1. Bar loaded in pure tension.

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an extrinsic property. For example, the introduction of carbon into iron modifies considerably the extent of the elastic region.

The extents of the elastic and plastic regions vary appreciably from one material to another. Fragile materials, for instance, have a much reduced plastic region, with a clear break.

#### 1.3.3.2. Elastic constants

##### 1.3.3.2.1. Definition

Young's modulus is not sufficient to describe the deformation of the bar: its diameter is reduced, in effect, during the elongation. One other coefficient, at least, is therefore necessary. In a general way, let us consider the deformation of a continuous anisotropic medium under the action of a field of applied stresses. We will generalize Hooke's law by writing that at each point there is a linear relation between the components  $T_{ij}$  of the stress tensor and the components  $S_{ij}$  of the strain tensor:

$$\begin{aligned} S_{ij} &= s_{ijkl} T_{kl} \\ T_{ij} &= c_{ijkl} S_{kl}. \end{aligned} \quad (1.3.3.2)$$

The quantities  $s_{ijkl}$  and  $c_{ijkl}$  are characteristic of the elastic properties of the medium if it is homogeneous and are independent of the point under consideration. Their tensorial nature can be shown using the demonstration illustrated in Section 1.1.3.4. Let us take the contracted product of the two sides of each of the two equations of (1.3.3.2) by the components  $x_i$  and  $y_j$  of any two vectors,  $\mathbf{x}$  and  $\mathbf{y}$ :

$$\begin{aligned} S_{ij} x_i y_j &= s_{ijkl} T_{kl} x_i y_j \\ T_{ij} x_i y_j &= c_{ijkl} S_{kl} x_i y_j. \end{aligned}$$

The left-hand sides are bilinear forms since  $S_{ij}$  and  $T_{ij}$  are second-rank tensors and the right-hand sides are quadrilinear forms, which shows that  $s_{ijkl}$  and  $c_{ijkl}$  are the components of fourth-rank tensors, the tensor of elastic *compliances* (or moduli) and the tensor of elastic *stiffnesses* (or coefficients), respectively. The number of their components is equal to 81.

Equations (1.3.3.2) are Taylor expansions limited to the first term. The higher terms involve sixth-rank tensors,  $s_{ijklmn}$  and  $c_{ijklmn}$ , with  $3^6 = 729$  coefficients, called third-order elastic compliances and stiffnesses and eighth-rank tensors with  $3^8 = 6561$  coefficients, called fourth-order elastic compliances and stiffnesses. They will be defined in Section 1.3.6.4. Tables for third-order elastic constants are given in Fumi (1951, 1952, 1987). The accompanying software to this volume enables these tables to be derived for any point group.

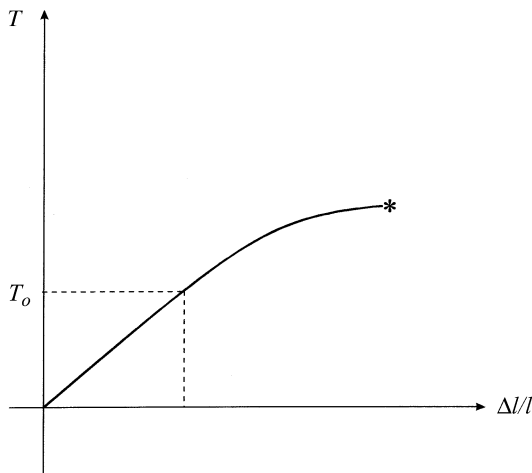


Fig. 1.3.3.2. Schematic stress-strain curve.  $T$ : stress;  $T_0$ : elastic limit;  $\Delta l/l$ : elongation; the asterisk symbolizes the rupture.

##### 1.3.3.2.2. Matrix notation – reduction of the number of independent components

It is convenient to write the relations (1.3.3.2) in matrix form by associating with the stress and strain tensors column matrices  $1 \times 9$  and with the tensors of the elastic stiffnesses,  $c$ , and of the elastic compliances,  $s$ , square matrices  $9 \times 9$  (Section 1.1.4.10.4); these two  $9 \times 9$  matrices are inverse to one another. The number of independent components of the fourth-rank elastic tensors can be reduced by three types of consideration:

(i) *Intrinsic symmetry*: it was shown in Section 1.1.1.4 that tensors representing principal properties are symmetric. This is the case of the elastic tensors and can be shown directly using expression (1.3.2.7) of the energy stored per unit volume in the medium when we allow it to deform from the state  $S_{ij}$  to the state  $S_{ij} + \delta S_{ij}$  under the action of the stress  $T_{ij}$ :

$$\delta W = T_{ij} \delta S_{ij}.$$

Applying relation (1.3.3.1), we get

$$\partial W / \partial S_{ij} = c_{ijkl} S_{kl}. \quad (1.3.3.3)$$

Hence, one has by further differentiation

$$\partial^2 W / (\partial S_{ij} \partial S_{kl}) = c_{ijkl}.$$

Nothing is changed by interchanging the role of the pairs of dummy indices  $ij$  and  $lk$ :

$$\partial^2 W / (\partial S_{kl} \partial S_{ij}) = c_{klij}.$$

Since the energy is a state function with a perfect differential, one can interchange the order of the differentiations: the members on the left-hand sides of these two equations are therefore equal; one then deduces

$$c_{ijkl} = c_{klij}. \quad (1.3.3.4)$$

The tensor of elastic stiffnesses (and also the tensor of elastic compliances) is thus symmetrical. As shown in Section 1.1.4.5.2.2, the number of their independent components is therefore reduced to 45.

(ii) *Symmetry of the strain and stress tensors*: the strain tensor  $S_{ij}$  is symmetric by definition (Section 1.3.1.3.1) because rotations are not taken into account and the stress tensor  $T_{ij}$  is symmetric (Section 1.3.2.4) because body torques are neglected. For this reason, summation (1.3.3.2),  $S_{ij} = s_{ijkl} T_{kl}$ , can be factorized [equation (1.1.4.11)]:

$$S_{ij} = \sum_l s_{ijll} T_{ll} + \sum_{k \neq l} (s_{ijkl} + s_{ijlk}) T_{kl}.$$

This shows that the number of independent components of tensor  $s_{ijkl}$  is reduced. This effect of the symmetry of the strain and stress tensors was discussed systematically in Section 1.1.4.10.4. It was shown that

$$\begin{aligned} s_{ijkl} &= s_{ijlk} = s_{jikl} = s_{jilk} \\ c_{ijkl} &= c_{ijlk} = c_{jikl} = c_{jilk} \end{aligned} \quad (1.3.3.5)$$

and that the number of independent elastic compliances or stiffnesses is reduced to 21. They are replaced by two-index coefficients constituting  $6 \times 6$  matrices according to Voigt's notation:

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

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

$$c_{ijkl} = c_{ikjl} = c_{iljk}$$

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
$4/mmm, 422, \bar{4}2m, 42m$	6
$6/m, 6, 6$	5
$6/mmm, 622, \bar{6}2m, 62m$	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,  $\chi$ , which is the inverse of the *bulk modulus*,  $\kappa$ :

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

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  $\alpha_i$ '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  $s_{11}$ ,  $s_{12}$ ,  $s_{44}$ ,  $\nu$  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)<sup>-1</sup> (after Landoldt-Börnstein, 1979)

Material	$s_{11}$	$s_{12}$	$s_{44}$	$\nu$	$s_{44}/2(s_{11} - s_{12})$
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 <sub>3</sub>	8.33	-2.68	9.24	0.322	0.420
Adamantane	240	-79	295	0.329	0.462
Almandine (Fe <sub>3</sub> Al <sub>2</sub> Si <sub>3</sub> O <sub>12</sub> )	4.036	-1.093	10.77	0.271	1.050
Spinel (MgAl <sub>2</sub> O <sub>4</sub> )	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  $\theta$  is the angle between  $Ox'_1$  and  $Ox_1$ , and  $\varphi$  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,  $\bar{3}$ ):

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

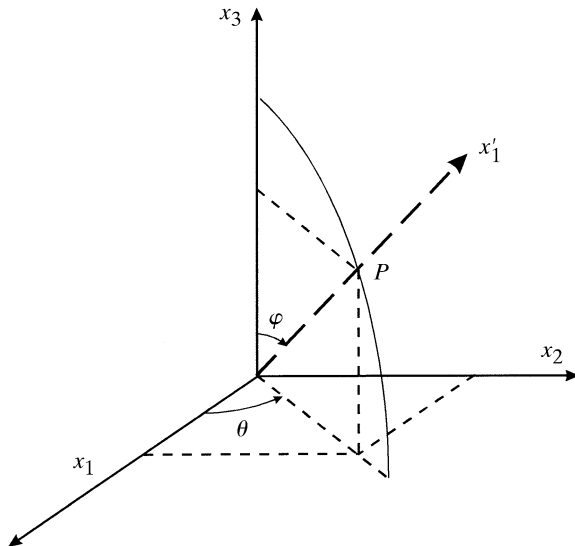


Fig. 1.3.3.3. Spherical coordinates.

(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

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

### 1.3. ELASTIC PROPERTIES

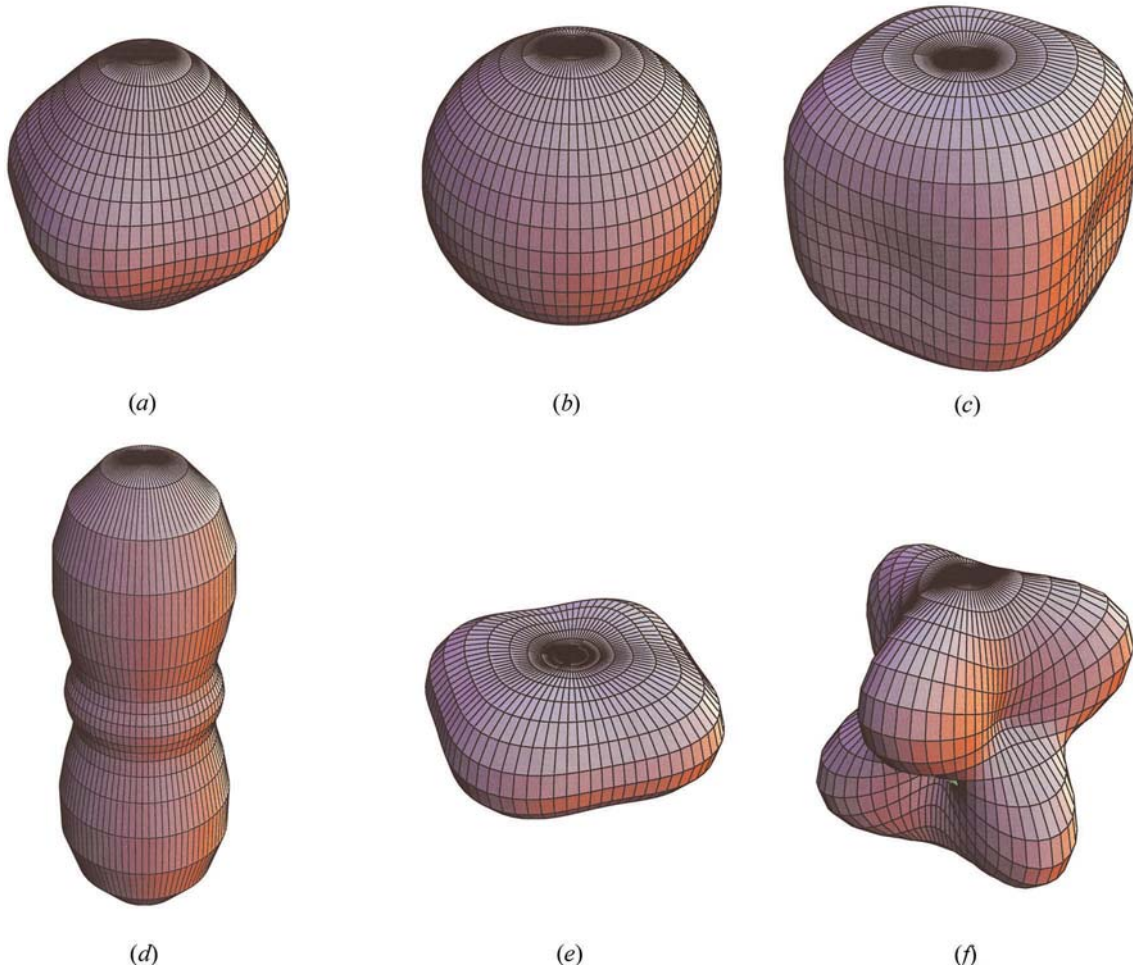


Fig. 1.3.3.4. Representation surface of the inverse of Young's modulus. (a) NaCl, cubic, anisotropy factor  $> 1$ ; (b) W, cubic, anisotropy factor  $= 1$ ; (c) Al, cubic, anisotropy factor  $< 1$ ; (d) Zn, hexagonal; (e) Sn, tetragonal; (f) calcite, trigonal.

If one introduces the Lamé constants,

$$\begin{aligned}\mu &= (1/2)(c_{11} - c_{12}) = c_{44} \\ \lambda &= c_{12},\end{aligned}$$

the equations may be written in the form often used in mechanics:

$$\begin{aligned}T_1 &= 2\mu S_1 + \lambda(S_1 + S_2 + S_3) \\ T_2 &= 2\mu S_2 + \lambda(S_1 + S_2 + S_3) \\ T_3 &= 2\mu S_3 + \lambda(S_1 + S_2 + S_3).\end{aligned}\quad (1.3.3.16)$$

Two coefficients suffice to define the elastic properties of an isotropic material,  $s_{11}$  and  $s_{12}$ ,  $c_{11}$  and  $c_{12}$ ,  $\mu$  and  $\lambda$ ,  $\mu$  and  $\nu$ , etc. Table 1.3.3.3 gives the relations between the more common elastic coefficients.

#### 1.3.3.6. Equilibrium conditions of elasticity for isotropic media

We saw in Section 1.3.2.3 that the condition of equilibrium is

$$\partial T_{ij} / \partial x_i + \rho F_j = 0.$$

If we use the relations of elasticity, equation (1.3.3.2), this condition can be rewritten as a condition on the components of the strain tensor:

$$c_{ijkl} \frac{\partial S_{kl}}{\partial x_j} + \rho F_i = 0.$$

Recalling that

$$S_{kl} = \frac{1}{2} \left[ \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right],$$

the condition becomes a condition on the displacement vector,  $\mathbf{u}(\mathbf{r})$ :

$$c_{ijkl} \frac{\partial^2}{\partial x_i \partial x_j} + \rho F_i = 0.$$

In an isotropic orthonormal medium, this equation, projected on the axis  $0x_1$ , can be written with the aid of relations (1.3.3.5) and (1.3.3.9):

$$\begin{aligned}& c_{11} \frac{\partial^2 u_1}{(\partial x_1)^2} + c_{12} \left[ \frac{\partial^2 u_2}{\partial x_1 \partial x_2} + \frac{\partial^2 u_3}{\partial x_1 \partial x_3} \right] \\ & + \frac{1}{2} (c_{11} - c_{12}) \left[ \frac{\partial^2 u_1}{(\partial x_2)^2} + \frac{\partial^2 u_3}{\partial x_1 \partial x_3} + \frac{\partial^2 u_1}{(\partial x_3)^2} \right] + \rho F_1 \\ & = 0.\end{aligned}$$

This equation can finally be rearranged in one of the three following forms with the aid of Table 1.3.3.3.

$$\begin{aligned}\frac{1}{2} (c_{11} - c_{12}) \Delta \mathbf{u} + \frac{1}{2} (c_{11} + c_{12}) \nabla (\nabla \cdot \mathbf{u}) + \rho \mathbf{F} &= 0 \\ \mu \Delta \mathbf{u} + (\mu + \lambda) \nabla (\nabla \cdot \mathbf{u}) + \rho \mathbf{F} &= 0 \\ \mu \left[ \Delta \mathbf{u} + \frac{1}{1 - 2\nu} \nabla (\nabla \cdot \mathbf{u}) \right] + \rho \mathbf{F} &= 0.\end{aligned}\quad (1.3.3.17)$$