

1.3. ELASTIC PROPERTIES

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

## 1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

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,  $\bar{3}$ ):

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

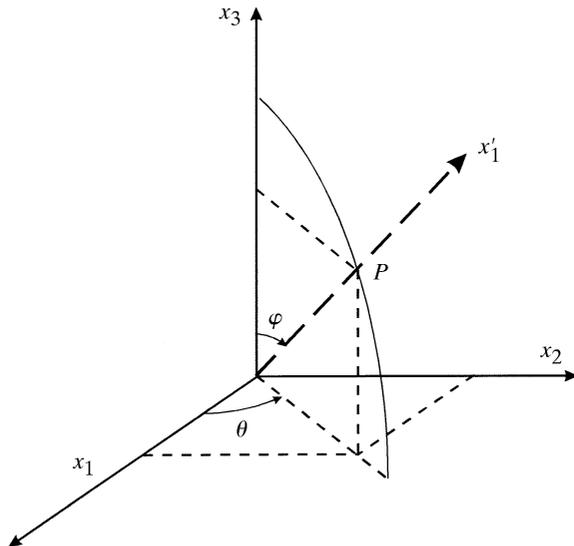


Fig. 1.3.3.3. Spherical coordinates.

(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

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