1.3. ELASTIC PROPERTIES

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:

$$S_{ij} = s_{ijkl} T_{kl}$$
$$T_{ij} = c_{ijkl} S_{kl}. \qquad (1.3.3.2)$$

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, **x** and **y**:

$$S_{ij} x_i y_j = s_{ijkl} T_{kl} x_i y_j$$
$$T_{ij} x_i y_j = c_{ijkl} S_{kl} x_i y_j.$$

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.
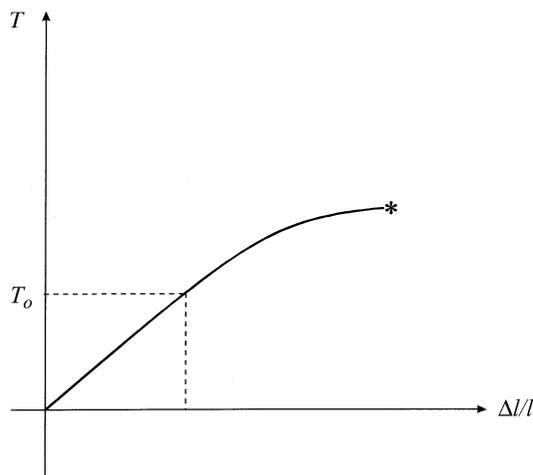

Fig. 1.3.3.2. Schematic stress–strain curve. T: stress; T_o: elastic limit; $\Delta l/l$: elongation; the asterisk symbolizes the rupture.

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 1×9 and with the tensors of the elastic stiffnesses, c, and of the elastic compliances, s, square matrices 9×9 (Section 1.1.4.10.4); these two 9×9 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}:

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

Applying relation (1.3.3.1), we get

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

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

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

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)]:

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

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

$$s_{ijkl} = s_{ijlk} = s_{jikl} = s_{jilk}$$
$$c_{ijkl} = c_{ijlk} = c_{jikl} = c_{jilk} \qquad (1.3.3.5)$$

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

$$
\left.\begin{array}{llll}
i = j; & k = l & s_{\alpha\beta} = siill \\
i = j; & k \neq l & s_{\alpha\beta} = siill + siilk \\
i \neq j; & k = l & s_{\alpha\beta} = sijll + sjill \\
i \neq j; & k \neq l & s_{\alpha\beta} = sijkl + sjikl + sijlk + sjilk
\end{array}\right\} \quad c_{\alpha\beta} = cijkl.
$$

$$(1.3.3.6)$$

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

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

$$(1.3.3.7)$$

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 another. 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:

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

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
$3m, 32, 3m$	6
$4/m, 4, \bar{4}$	7
$4/mmm, 422, \bar{4}2m, 42m$	6
$6/m, 6, \bar{6}$	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:

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

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

where we have, for isotropic materials,

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

$$(1.3.3.9)$$

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

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

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