International Tables for Crystallography (2006). Vol. D, Section 1.3.3.1, pp. 80–81.

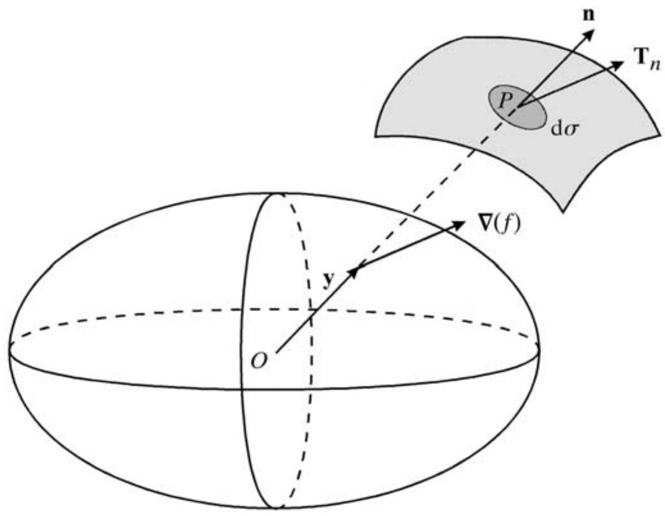

Fig. 1.3.2.7. The stress quadric: application to the determination of the stress applied to a surface element. The surface of the medium is shaded in light grey and a small surface element, dσ, is shaded in medium grey. The stress at P is proportional to $\nabla(f)$ at the intersection of **OP** with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

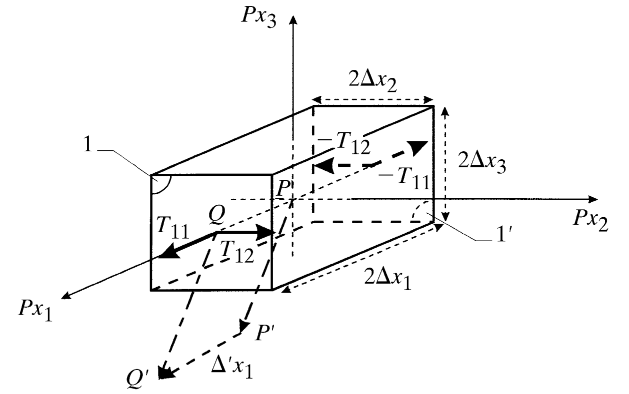

Fig. 1.3.2.8. Determination of the energy density in a deformed medium. **PP′** represents the displacement of the small parallelepiped during the deformation. The thick arrows represent the forces applied to the faces 1 and 1′.

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

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

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

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

$$\delta W = T_{ij} \delta S_{ji}. \qquad (1.3.2.7)$$

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 $T = F/\mathcal{A}$ (F applied force, $\mathcal{A}$ 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 Δl 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*:

$$\frac{\Delta l}{l} = \frac{1}{E} T, \qquad (1.3.3.1)$$

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

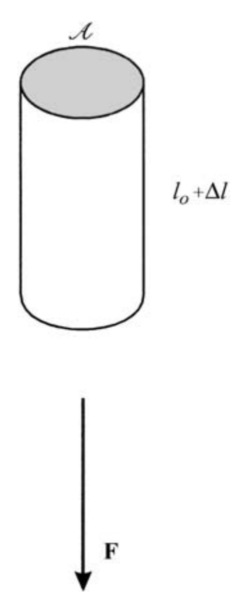

Fig. 1.3.3.1. Bar loaded in pure tension.

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:

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

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, $\mathbf{x}$ 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.

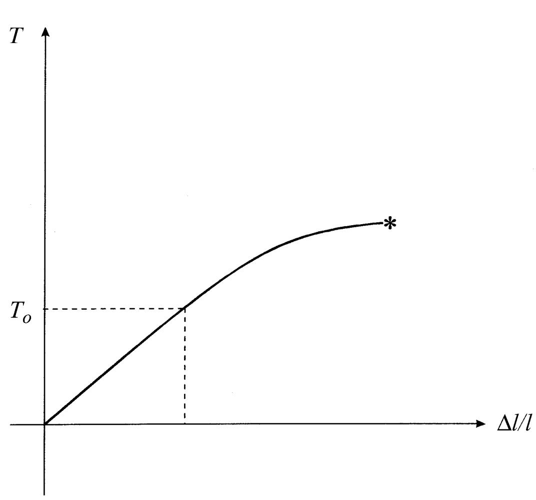

Fig. 1.3.3.2. Schematic stress–strain curve. T: stress; T_o: elastic limit; $\Delta l/l$: elongation; the asterisk symbolizes the rupture.

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

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

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: