

1.3. Elastic properties

BY A. AUTHIER AND A. ZAREMBOWITCH

1.3.1. Strain tensor

1.3.1.1. Introduction, the notion of strain field

Let us consider a medium that undergoes a deformation. This means that the various points of the medium are displaced with respect to one another. Geometrical transformations of the medium that reduce to a translation of the medium as a whole will therefore not be considered. We may then suppose that there is an invariant point, O , whose position one can always return to by a suitable translation. A point P , with position vector $\mathbf{OP} = \mathbf{r}$, is displaced to the neighbouring point P' by the deformation defined by

$$\mathbf{PP}' = \mathbf{u}(\mathbf{r}).$$

The displacement vector $\mathbf{u}(\mathbf{r})$ constitutes a vector field. It is not a uniform field, unless the deformation reduces to a translation of the whole body, which is incompatible with the hypothesis that the medium undergoes a deformation. Let Q be a point that is near P before the deformation (Fig. 1.3.1.1). Then one can write

$$\mathbf{dr} = \mathbf{PQ}; \quad \mathbf{r} + \mathbf{dr} = \mathbf{OQ}.$$

After the deformation, Q is displaced to Q' defined by

$$\mathbf{QQ}' = \mathbf{u}(\mathbf{r} + \mathbf{dr}).$$

In a deformation, it is more interesting in general to analyse the local, or relative, deformation than the absolute displacement. The relative displacement is given by comparing the vectors $\mathbf{P'Q}' = \mathbf{dr}'$ and \mathbf{PQ} . Thus, one has

$$\mathbf{P'Q}' = \mathbf{P'P} + \mathbf{PQ} + \mathbf{QQ}'.$$

Let us set

$$\left. \begin{aligned} \mathbf{dr}' &= \mathbf{dr} + \mathbf{u}(\mathbf{r} + \mathbf{dr}) - \mathbf{u}(\mathbf{r}) \\ \mathbf{du} &= \mathbf{u}(\mathbf{r} + \mathbf{dr}) - \mathbf{u}(\mathbf{r}) = \mathbf{dr}' - \mathbf{dr}. \end{aligned} \right\} \quad (1.3.1.1)$$

Replacing $\mathbf{u}(\mathbf{r} + \mathbf{dr})$ by its expansion up to the first term gives

$$\left. \begin{aligned} \mathbf{du}_i &= \frac{\partial u_i}{\partial x_j} dx_j \\ \mathbf{dx}'_i &= dx_i + \frac{\partial u_i}{\partial x_j} dx_j. \end{aligned} \right\} \quad (1.3.1.2)$$

If we assume the Einstein convention (see Section 1.1.2.1), there is summation over j in (1.3.1.2) and (1.3.1.3). We shall further assume orthonormal coordinates throughout Chapter 1.3; variance is therefore not apparent and the positions of the indices have no meaning; the Einstein convention then only assumes repetition of a dummy index. The elements dx_i and dx'_i are the components of \mathbf{dr} and \mathbf{dr}' , respectively. Let us put

$$M_{ij} = \partial u_i / \partial x_j; \quad B_{ij} = M_{ij} + \delta_{ij},$$

where δ_{ij} represents the Kronecker symbol; the δ_{ij} 's are the components of matrix unity, I . The expressions (1.3.1.2) can also be written using matrices M and B :

$$\left. \begin{aligned} \mathbf{du}_i &= M_{ij} dx_j \\ \mathbf{dx}'_i &= B_{ij} dx_j. \end{aligned} \right\} \quad (1.3.1.3)$$

The components of the tensor M_{ij} are nonzero, unless, as mentioned earlier, the deformation reduces to a simple translation. Two cases in particular are of interest and will be discussed in turn:

- (i) The components M_{ij} are constants. In this case, the deformation is homogeneous.
- (ii) The components M_{ij} are variables but are small compared with unity. This is the practical case to which we shall limit ourselves in considering an inhomogeneous deformation.

1.3.1.2. Homogeneous deformation

If the components M_{ij} are constants, equations (1.3.1.3) can be integrated directly. They become, to a translation,

$$\left. \begin{aligned} u_i &= M_{ij} x_j \\ x'_i &= B_{ij} x_j. \end{aligned} \right\} \quad (1.3.1.4)$$

1.3.1.2.1. Fundamental property of the homogeneous deformation

The fundamental property of the homogeneous deformation results from the fact that equations (1.3.1.4) are linear: a plane before the deformation remains a plane afterwards, a crystal lattice remains a lattice. Thermal expansion is a homogeneous deformation (see Chapter 1.4).

1.3.1.2.2. Spontaneous strain

Some crystals present a twin microstructure that is seen to change when the crystals are gently squeezed. At rest, the domains can have one of two different possible orientations and the influence of an applied stress is to switch them from one orientation to the other. If one measures the shape of the crystal lattice (the strain of the lattice) as a function of the applied stress, one obtains an elastic hysteresis loop analogous to the magnetic or electric hysteresis loops observed in ferromagnetic or ferroelectric crystals. For this reason, these materials are called *ferroelastic* (see Chapters 3.1 to 3.3 and Salje, 1990). The strain associated with one of the two possible shapes of the crystal when no stress is applied is called the macroscopic *spontaneous strain*.

1.3.1.2.3. Cubic dilatation

Let \mathbf{e}_i be the basis vectors before deformation. On account of the deformation, they are transformed into the three vectors

$$\mathbf{e}'_i = B_{ij} \mathbf{e}_j.$$

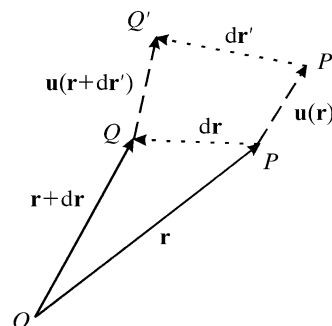


Fig. 1.3.1.1. Displacement vector, $\mathbf{u}(\mathbf{r})$.

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The parallelepiped formed by these three vectors has a volume V' given by

$$V' = (\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3) = \Delta(B)(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3) = \Delta(B)V,$$

where $\Delta(B)$ is the determinant associated with matrix B , V is the volume before deformation and

$$(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3) = (\mathbf{e}_1 \wedge \mathbf{e}_2) \cdot \mathbf{e}_3$$

represents a triple scalar product.

The relative variation of the volume is

$$\frac{V' - V}{V} = \Delta(B) - 1. \quad (1.3.1.5)$$

It is what one calls the *cubic dilatation*. $\Delta(B)$ gives directly the volume of the parallelepiped that is formed from the three vectors obtained in the deformation when starting from vectors forming an orthonormal base.

1.3.1.2.4. *Expression of any homogeneous deformation as the product of a pure rotation and a pure deformation*

(i) *Pure rotation*: It is isometric. The moduli of the vectors remain unchanged and one direction remains invariant, the axis of rotation. The matrix B is unitary:

$$BB^T = 1.$$

(ii) *Pure deformation*: This is a deformation in which three orthogonal directions remain invariant. It can be shown that B is a symmetric matrix:

$$B = B^T.$$

The three invariant directions are those of the eigenvectors of the matrix; it is known in effect that the eigenvectors of a symmetric matrix are real.

(iii) *Arbitrary deformation*: the matrix B , representing an arbitrary deformation, can always be put into the form of the product of a unitary matrix B_1 , representing a pure rotation, and a symmetric matrix B_2 , representing a pure deformation. Let us put

$$B = B_1 B_2$$

and consider the transpose matrix of B :

$$B^T = B_2^T B_1^T = B_2 (B_1)^{-1}.$$

The product $B^T B$ is equal to

$$B^T B = (B_2)^2.$$

This shows that we can determine B_2 and therefore B_1 from B .

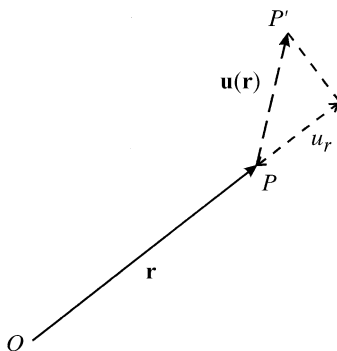


Fig. 1.3.1.2. Elongation, u_r/r .

1.3.1.2.5. *Quadric of elongations*

Let us project the displacement vector $\mathbf{u}(\mathbf{r})$ on the position vector \mathbf{OP} (Fig. 1.3.1.2), and let u_r be this projection. The *elongation* is the quantity defined by

$$\frac{u_r}{r} = \frac{\mathbf{u} \cdot \mathbf{r}}{r^2} = \frac{M_{ij} x_i x_j}{r^2},$$

where x_1, x_2, x_3 are the components of \mathbf{r} . The elongation is the relative variation of the length of the vector \mathbf{r} in the deformation. Let A and S be the antisymmetric and symmetric parts of M , respectively:

$$A = \frac{M - M^T}{2}; \quad S = \frac{M + M^T}{2}.$$

Only the symmetric part of M occurs in the expression of the elongation:

$$\frac{u_r}{r} = \frac{S_{ij} x_i x_j}{r^2}. \quad (1.3.1.6)$$

The geometrical study of the elongation as a function of the direction of \mathbf{r} is facilitated by introducing the quadric associated with M :

$$S_{ij} y_i y_j = \varepsilon, \quad (1.3.1.7)$$

where ε is a constant. This quadric is called the *quadric of elongations*, Q . S is a symmetric matrix with three real orthogonal eigenvectors and three real eigenvalues, $\lambda_1, \lambda_2, \lambda_3$. If it is referred to these axes, equation (1.3.1.7) is reduced to

$$\lambda_1 (y_1)^2 + \lambda_2 (y_2)^2 + \lambda_3 (y_3)^2 = \varepsilon.$$

One can discuss the form of the quadric according to the sign of the eigenvalues λ_i :

(i) $\lambda_1, \lambda_2, \lambda_3$ have the same sign, and the sign of ε . The quadric is an ellipsoid (Fig. 1.3.1.3a). One chooses $\varepsilon = +1$ or $\varepsilon = -1$, depending on the sign of the eigenvalues.

(ii) $\lambda_1, \lambda_2, \lambda_3$ are of mixed signs: one of them is of opposite sign to the other two. One takes $\varepsilon = \pm 1$. The corresponding quadric is a hyperboloid whose asymptote is the cone

$$S_{ij} y_i y_j = 0.$$

According to the sign of ε , the hyperboloid will have one sheet outside the cone or two sheets inside the cone (Fig. 1.3.1.3b). If we wish to be able to consider any direction of the position vector \mathbf{r} in space, it is necessary to take into account the two quadrics.

In order to follow the variations of the elongation u_r/r with the orientation of the position vector, one associates with \mathbf{r} a vector \mathbf{y} , which is parallel to it and is defined by

$$\mathbf{y} = \mathbf{r}/k; \quad \mathbf{r} = k\mathbf{y},$$

where k is a constant. It can be seen that, in accordance with (1.3.1.6) and (1.3.1.7), the expression of the elongation in terms of \mathbf{y} is

$$u_r/r = \varepsilon/y^2.$$

Thus, the elongation is inversely proportional to the square of the radius vector of the quadric of elongations parallel to \mathbf{OP} . In practice, it is necessary to look for the intersection p of the parallel to \mathbf{OP} drawn from the centre O of the quadric of elongations (Fig. 1.3.1.3a):

(i) The eigenvalues all have the same sign; the quadric Q is an ellipsoid: the elongation has the same sign in all directions in space, positive for $\varepsilon = +1$ and negative for $\varepsilon = -1$.

(ii) The eigenvalues have different signs; two quadrics are to be taken into account: the hyperboloids corresponding, respectively, to $\varepsilon = \pm 1$. The sign of the elongation is different according to

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whether the direction under consideration is outside or inside the asymptotic cone and intersects one or the other of the two hyperboloids.

Equally, one can connect the displacement vector $\mathbf{u}(\mathbf{r})$ directly with the quadric Q . Using the bilinear form

$$f(\mathbf{y}) = M_{ij}y_iy_j,$$

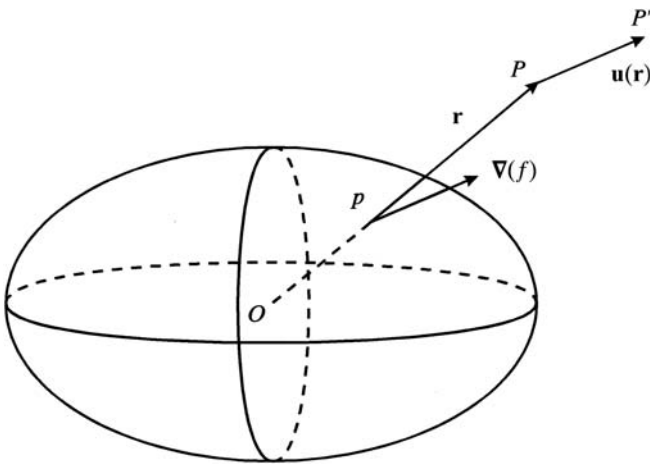
the gradient of $f(\mathbf{y})$, $\nabla(f)$, has as components

$$\partial f / \partial y^i = M_{ij}y_j = u_i.$$

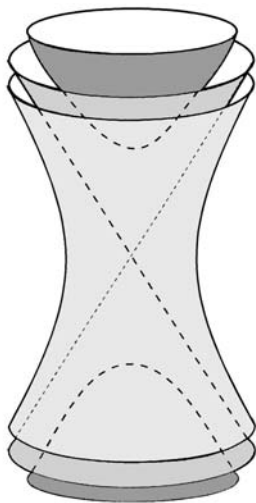
One recognizes the components of the displacement vector \mathbf{u} , which is therefore parallel to the normal to the quadric Q at the extremity of the radius vector \mathbf{Op} parallel to \mathbf{r} .

The directions of the principal axes of Q correspond to the extremal values of y , *i.e.* to the stationary values (maximal or minimal) of the elongation. These values are the *principal elongations*.

If the deformation is a pure rotation



(a)



(b)

Fig. 1.3.1.3. Quadric of elongations. The displacement vector, $\mathbf{u}(\mathbf{r})$, at P in the deformed medium is parallel to the normal to the quadric at the intersection, p , of \mathbf{Op} with the quadric. (a) The eigenvalues all have the same sign, the quadric is an ellipsoid. (b) The eigenvalues have mixed signs, the quadric is a hyperboloid with either one sheet (shaded in light grey) or two sheets (shaded in dark grey), depending on the sign of the constant ε [see equation (1.3.1.7)]; the cone asymptote is represented in medium grey. For a practical application, see Fig. 1.4.1.1.

$$B = \begin{pmatrix} \cos \theta & \sin \theta & 0 \\ -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$M = \begin{pmatrix} \cos \theta - 1 & \sin \theta & 0 \\ -\sin \theta & \cos \theta - 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Hence we have

$$M_{ij}y_iy_j = (\cos \theta - 1)(y_1 - y_2) = \varepsilon.$$

The quadric Q is a cylinder of revolution having the axis of rotation as axis.

1.3.1.3. Arbitrary but small deformations

1.3.1.3.1. Definition of the strain tensor

If the deformation is small but arbitrary, *i.e.* if the products of two or more components of M_{ij} can be neglected with respect to unity, one can describe the deformation locally as a homogeneous asymptotic deformation. As was shown in Section 1.3.1.2.4, it can be put in the form of the product of a pure deformation corresponding to the symmetric part of M_{ij} , S_{ij} , and a pure rotation corresponding to the asymmetric part, A_{ij} :

$$\left. \begin{aligned} S_{ij} = S_{ji} &= \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \\ A_{ij} = -A_{ji} &= \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) \end{aligned} \right\} \quad (1.3.1.8)$$

Matrix B can be written

$$B = I + A + S,$$

where I is the matrix identity. As the coefficients $\partial u_i / \partial x_j$ of M_{ij} are small, one can neglect the product $A \times S$ and one has

$$B = (I + A)(I + S).$$

$(I + S)$ is a symmetric matrix that represents a pure deformation. $(I + A)$ is an antisymmetric unitary matrix and, since A is small,

$$(I + A)^{-1} = (I - A).$$

Thus, $(I + A)$ represents a rotation. The axis of rotation is parallel to the vector with coordinates

$$\left. \begin{aligned} \Omega_1 &= \frac{1}{2} \left(\frac{\partial u_3}{\partial x_2} + \frac{\partial u_2}{\partial x_3} \right) = A_{32} \\ \Omega_2 &= \frac{1}{2} \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \right) = A_{13} \\ \Omega_3 &= \frac{1}{2} \left(\frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2} \right) = A_{21}, \end{aligned} \right\}$$

which is an eigenvector of $(I + A)$. The magnitude of the rotation is equal to the modulus of this vector.

In general, one is only interested in the pure deformation, *i.e.* in the form of the deformed object. Thus, one only wishes to know the quantities $(I + S)$ and the symmetric part of M . It is this symmetric part that is called the deformation tensor or the strain tensor. It is very convenient for applications to use the simplified notation due to Voigt:

$$\begin{aligned} S_1 &= \frac{\partial u_1}{\partial x_1}; & S_2 &= \frac{\partial u_2}{\partial x_2}; & S_3 &= \frac{\partial u_3}{\partial x_3}; \\ S_4 &= \frac{\partial u_3}{\partial x_2} + \frac{\partial u_2}{\partial x_3}; & S_5 &= \frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}; & S_6 &= \frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2}. \end{aligned}$$

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One may note that

$$\begin{aligned} S_1 &= S_{11}; & S_2 &= S_{22}; & S_3 &= S_{33}; \\ S_4 &= S_{23} + S_{32}; & S_5 &= S_{31} + S_{13}; & S_6 &= S_{12} + S_{21}. \end{aligned}$$

The Voigt strain matrix S is of the form

$$\begin{pmatrix} S_1 & S_6 & S_5 \\ S_6 & S_2 & S_4 \\ S_5 & S_4 & S_3 \end{pmatrix}.$$

1.3.1.3.2. Geometrical interpretation of the coefficients of the strain tensor

Let us consider an orthonormal system of axes with centre P . We remove nothing from the generality of the following by limiting ourselves to a planar problem and assuming that point P' to which P goes in the deformation lies in the plane x_1Px_2 (Fig. 1.3.1.4). Let us consider two neighbouring points, Q and R , lying on axes Px_1 and Px_2 , respectively ($PQ = dx_1$, $PR = dx_2$). In the deformation, they go to points Q' and R' defined by

$$\begin{aligned} \mathbf{QQ}' : & \begin{cases} dx'_1 = dx_1 + (\partial u_1/\partial x_1)dx_1 \\ dx'_2 = (\partial u_2/\partial x_1)dx_1 \\ dx'_3 = 0 \end{cases} \\ \mathbf{RR}' : & \begin{cases} dx'_1 = (\partial u_1/\partial x_2)dx_2 \\ dx'_2 = dx_2 + (\partial u_2/\partial x_2)dx_2 \\ dx'_3 = 0. \end{cases} \end{aligned}$$

As the coefficients $\partial u_i/\partial x_j$ are small, the lengths of $P'Q'$ and $P'R'$ are hardly different from PQ and PR , respectively, and the elongations in the directions Px_1 and Px_2 are

$$\begin{aligned} \frac{P'Q' - PQ}{PQ} &= \frac{dx'_1 - dx_1}{dx_1} = \frac{\partial u_1}{\partial x_1} = S_1 \\ \frac{P'R' - PR}{PR} &= \frac{dx'_2 - dx_2}{dx_2} = \frac{\partial u_2}{\partial x_2} = S_2. \end{aligned}$$

The components S_1, S_2, S_3 of the principal diagonal of the Voigt matrix can then be interpreted as the elongations in the three directions Px_1, Px_2 and Px_3 . The angles α and β between \mathbf{PQ} and $\mathbf{P'Q'}$, and \mathbf{PR} and $\mathbf{P'R'}$, respectively, are given in the same way by

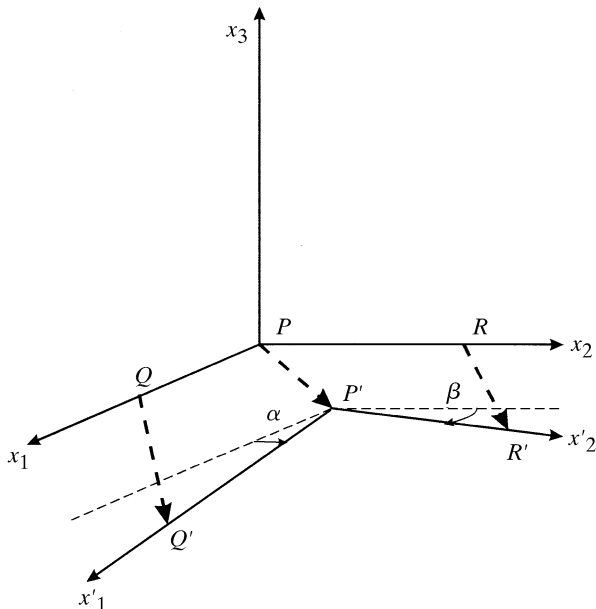


Fig. 1.3.1.4. Geometrical interpretation of the components of the strain tensor. Ox_1, Ox_2, Ox_3 : axes before deformation; Ox'_1, Ox'_2, Ox'_3 : axes after deformation.

$$\alpha = dx'_2/dx_1 = \partial u_2/\partial x_1; \quad \beta = dx'_1/dx_2 = \partial u_1/\partial x_2.$$

One sees that the coefficient S_6 of Voigt's matrix is therefore

$$S_6 = \frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2} = \alpha + \beta.$$

The angle $\alpha + \beta$ is equal to the difference between angles $\mathbf{PQ} \wedge \mathbf{PR}$ before deformation and $\mathbf{P'Q'} \wedge \mathbf{P'R'}$ after deformation. The nondiagonal terms of the Voigt matrix therefore represent the shears in the planes parallel to Px_1, Px_2 and Px_3 , respectively.

To summarize, if one considers a small cube before deformation, it becomes after deformation an arbitrary parallelepiped; the relative elongations of the three sides are given by the diagonal terms of the strain tensor and the variation of the angles by its nondiagonal terms.

The cubic dilatation (1.3.1.5) is

$$\Delta(B) - 1 = S_1 + S_2 + S_3$$

(taking into account the fact that the coefficients S_{ij} are small).

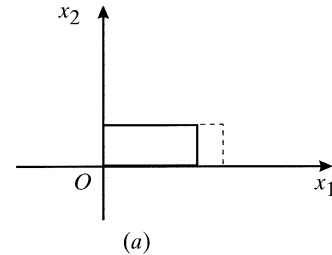
1.3.1.4. Particular components of the deformation

1.3.1.4.1. Simple elongation

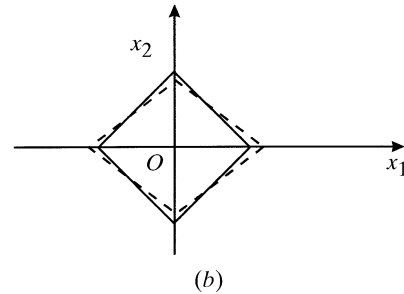
Matrix M has only one coefficient, e_1 , and reduces to (Fig. 1.3.1.5a)

$$\begin{pmatrix} e_1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

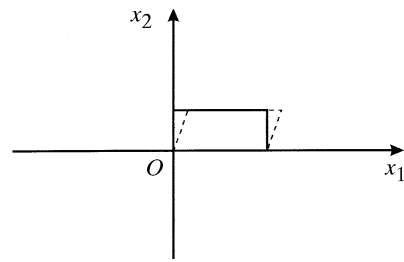
The quadric of elongations is reduced to two parallel planes, perpendicular to Ox_1 , with the equation $x_1 = \pm 1/\sqrt{|e_1|}$.



(a)



(b)



(c)

Fig. 1.3.1.5. Special deformations. The state after deformation is represented by a dashed line. (a) Simple elongation; (b) pure shear; (c) simple shear.

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1.3.1.4.2. Pure shear

This is a pure deformation (without rotation) consisting of the superposition of two simple elongations along two perpendicular directions (Fig. 1.3.1.5b) and such that there is no change of volume (the cubic dilatation is zero):

$$\begin{pmatrix} e_1 & 0 & 0 \\ 0 & -e_1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The quadric of elongations is a hyperbolic cylinder.

1.3.1.4.3. Simple shear

Matrix M_{ij} has one coefficient only, a shear (Fig. 1.3.1.5c):

$$\begin{pmatrix} 0 & s & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The matrix is not symmetrical, as it contains a component of rotation. Thus we have

$$\left. \begin{aligned} x'_1 &= x_1 + sx_2 \\ x'_2 &= x_2 \\ x'_3 &= x_3. \end{aligned} \right\}$$

One can show that the deformation is a pure shear associated with a rotation around Ox_3 .

1.3.2. Stress tensor

1.3.2.1. General conditions of equilibrium of a solid

Let us consider a solid C , in movement or not, with a mass distribution defined by a specific mass ρ at each point. There are two types of force that are manifested in the interior of this solid.

(i) *Body forces* (or mass forces), which one can write in the form

$$\mathbf{F} dm = \mathbf{F}\rho d\tau,$$

where $d\tau$ is a volume element and dm a mass element. Gravity forces or inertial forces are examples of body forces. One can also envisage body torques (or volume couples), which can arise, for example, from magnetic or electric actions but which will be seen to be neglected in practice.

(ii) *Surface forces or stresses*. Let us imagine a cut in the solid along a surface element $d\sigma$ of normal \mathbf{n} (Fig. 1.3.2.1). The two lips of the cut that were in equilibrium are now subjected to equal and opposite forces, \mathbf{R} and $\mathbf{R}' = -\mathbf{R}$, which will tend to separate or draw together these two lips. One admits that, when the area element $d\sigma$ tends towards zero, the ratio $\mathbf{R}/d\sigma$ tends towards a finite limit, \mathbf{T}_n , which is called *stress*. It is a force per unit area of surface, homogeneous to a pressure. It will be considered as positive if it is oriented towards the same side of the surface-area element $d\sigma$ as the normal \mathbf{n} and negative in the other case. The choice of the orientation of \mathbf{n} is arbitrary. The pressure in a liquid is defined in a similar way but its magnitude is independent of the orientation of \mathbf{n} and its direction is always parallel to \mathbf{n} . On the other hand, in a solid the constraint \mathbf{T}_n applied to a surface element is not necessarily normal to the latter and the magnitude and the orientation with respect to the normal change when the orientation of \mathbf{n} changes. A stress is said to be *homogeneous* if the force per unit area acting on a surface element of given orientation and given shape is independent of the position of the element in the body. Other stresses are *inhomogeneous*. Pressure is represented by a scalar, and stress by a rank-two tensor, which will be defined in Section 1.3.2.2.

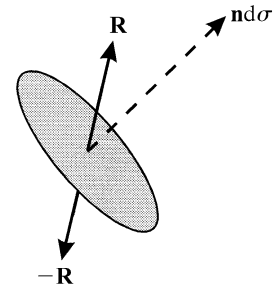


Fig. 1.3.2.1. Definition of stress: it is the limit of $\mathbf{R} d\sigma$ when the surface element $d\sigma$ tends towards zero. \mathbf{R} and \mathbf{R}' are the forces to which the two lips of the small surface element cut within the medium are subjected.

Now consider a volume V within the solid C and the surface S which surrounds it (Fig. 1.3.2.2). Among the influences that are exterior to V , we distinguish those that are external to the solid C and those that are internal. The first are translated by the body forces, eventually by volume couples. The second are translated by the local contact forces of the part external to V on the internal part; they are represented by a surface density of forces, *i.e.* by the stresses \mathbf{T}_n that depend only on the point Q of the surface S where they are applied and on the orientation of the normal \mathbf{n} of this surface at this point. If two surfaces S and S' are tangents at the same point Q , the same stress acts at the point of contact between them. The equilibrium of the volume V requires:

(i) For the resultant of the applied forces and the inertial forces:

$$\int_S \mathbf{T}_n d\sigma + \int_V \mathbf{F}\rho d\tau = \frac{d}{dt} \left\{ \int_V \mathbf{v} d\tau \right\}. \quad (1.3.2.1)$$

(ii) For the resultant moment:

$$\int_S \mathbf{OQ} \wedge \mathbf{T}_n d\sigma + \int_V \mathbf{OP} \wedge \mathbf{F}\rho d\tau = \frac{d}{dt} \left\{ \int_V \mathbf{OP} \wedge \mathbf{v} d\tau \right\}, \quad (1.3.2.2)$$

where Q is a point on the surface S , P a point in the volume V and \mathbf{v} the velocity of the volume element $d\tau$.

The equilibrium of the solid C requires that:

- (i) there are no stresses applied on its surface and
- (ii) the above conditions are satisfied for *any* volume V within the solid C .

1.3.2.2. Definition of the stress tensor

Using the condition on the resultant of forces, it is possible to show that the components of the stress \mathbf{T}_n can be determined from the knowledge of the orientation of the normal \mathbf{n} and of the components of a rank-two tensor. Let P be a point situated inside volume V , Px_1 , Px_2 and Px_3 three orthonormal axes, and consider a plane of arbitrary orientation that cuts the three axes at Q , R

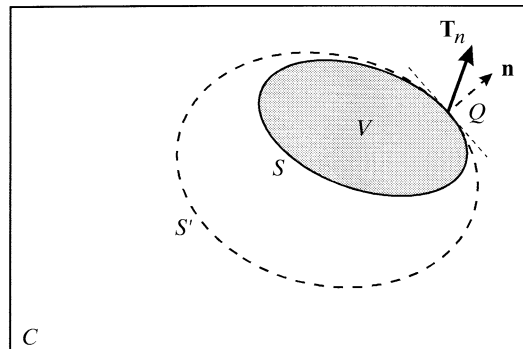


Fig. 1.3.2.2. Stress, \mathbf{T}_n , applied to the surface of an internal volume.

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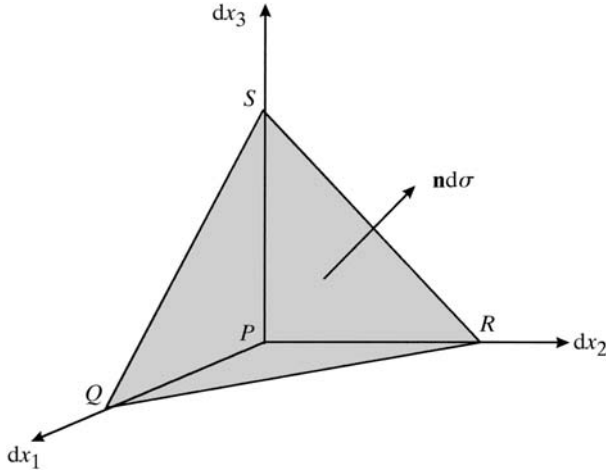


Fig. 1.3.2.3. Equilibrium of a small volume element.

and S , respectively (Fig. 1.3.2.3). The small volume element $PQRS$ is limited by four surfaces to which stresses are applied. The normals to the surfaces PRS , PSQ and PQR will be assumed to be directed towards the interior of the small volume. By contrast, for reasons that will become apparent later, the normal \mathbf{n} applied to the surface QRS will be oriented towards the exterior. The corresponding applied forces are thus given in Table 1.3.2.1. The volume $PQRS$ is subjected to five forces: the forces applied to each surface and the resultant of the volume forces and the inertial forces. The equilibrium of the small volume requires that the resultant of these forces be equal to zero and one can write

$$-\mathbf{T}_n d\sigma + \mathbf{T}_1 d\sigma_1 + \mathbf{T}_2 d\sigma_2 + \mathbf{T}_3 d\sigma_3 + \mathbf{F}\rho d\tau = 0$$

(including the inertial forces in the volume forces).

As long as the surface element $d\sigma$ is finite, however small, it is possible to divide both terms of the equation by it. If one introduces the direction cosines, α_i , the equation becomes

$$-\mathbf{T}_n + \mathbf{T}_1 d\alpha_1 + \mathbf{T}_2 d\alpha_2 + \mathbf{T}_3 d\alpha_3 + \mathbf{F}\rho d\tau/d\sigma = 0.$$

When $d\sigma$ tends to zero, the ratio $d\sigma/d\tau$ tends towards zero at the same time and may be neglected. The relation then becomes

$$\mathbf{T}_n = \mathbf{T}_i \alpha^i. \quad (1.3.2.3)$$

This relation is called the Cauchy relation, which allows the stress \mathbf{T}_n to be expressed as a function of the stresses \mathbf{T}_1 , \mathbf{T}_2 and \mathbf{T}_3 that are applied to the three faces perpendicular to the axes, Px_1 , Px_2 and Px_3 . Let us project this relation onto these three axes:

$$T_{nj} = T_{ij} \alpha^i. \quad (1.3.2.4)$$

The nine components T_{ij} are, by definition, the components of the stress tensor. In order to check that they are indeed the components of a tensor, it suffices to make the contracted product of each side of (1.3.2.4) by any vector x_i : the left-hand side is a scalar product and the right-hand side a bilinear form. The T_{ij} 's are therefore the components of a tensor. The index to the far left indicates the face to which the stress is applied (normal to the x_1 , x_2 or x_3 axis), while the second one indicates on which axis the stress is projected.

Table 1.3.2.1. Stresses applied to the faces surrounding a volume element

α_1 , α_2 and α_3 are the direction cosines of the normal \mathbf{n} to the small surface QRS .

Face	Area	Applied stress	Applied force
QRS	$d\sigma$	$-\mathbf{T}_n$	$-\mathbf{T}_n d\sigma$
PRS	$d\sigma_1 = \alpha_1 d\sigma$	\mathbf{T}_1	$\mathbf{T}_1 d\sigma_1$
PSQ	$d\sigma_2 = \alpha_2 d\sigma$	\mathbf{T}_2	$\mathbf{T}_2 d\sigma_2$
PQR	$d\sigma_3 = \alpha_3 d\sigma$	\mathbf{T}_3	$\mathbf{T}_3 d\sigma_3$

1.3.2.3. Condition of continuity

Let us return to equation (1.3.2.1) expressing the equilibrium condition for the resultant of the forces. By replacing \mathbf{T}_n by the expression (1.3.2.4), we get, after projection on the three axes,

$$\int_S \int T_{ij} d\sigma_i + \int_V \int F_j \rho d\tau = 0,$$

where $d\sigma_i = \alpha_i d\sigma$ and the inertial forces are included in the volume forces. Applying Green's theorem to the first integral, we have

$$\int_S \int T_{ij} d\sigma_i = \int_V \int [\partial T_{ij} / \partial x_i] d\tau.$$

The equilibrium condition now becomes

$$\int_V \int [\partial T_{ij} / \partial x_i + F_j \rho] d\tau = 0.$$

In order that this relation applies to any volume V , the expression under the integral must be equal to zero,

$$\partial T_{ij} / \partial x_i + F_j \rho = 0, \quad (1.3.2.5)$$

or, if one includes explicitly the inertial forces,

$$\partial T_{ij} / \partial x_i + F_j \rho = -\rho \partial^2 x_j / \partial t^2. \quad (1.3.2.6)$$

This is the condition of continuity or of conservation. It expresses how constraints propagate throughout the solid. This is how the cohesion of the solid is ensured. The resolution of any elastic problem requires solving this equation in terms of the particular boundary conditions of that problem.

1.3.2.4. Symmetry of the stress tensor

Let us now consider the equilibrium condition (1.3.2.2) relative to the resultant moment. After projection on the three axes, and using the Cartesian expression (1.1.3.4) of the vectorial products, we obtain

$$\int_S \int \frac{1}{2} \varepsilon_{ijk} (x_i T_{lj} - x_j T_{li}) d\sigma_l + \int_V \int \left[\frac{1}{2} \varepsilon_{ijk} \rho (x_i F_j - x_j F_i) + \Gamma_k \right] d\tau = 0.$$

(including the inertial forces in the volume forces). ε_{ijk} is the permutation tensor. Applying Green's theorem to the first integral and putting the two terms together gives

$$\int_V \int \left\{ \frac{1}{2} \varepsilon_{ijk} \left[\frac{\partial}{\partial x_l} (x_i T_{lj} - x_j T_{li}) + \rho (x_i F_j - x_j F_i) \right] + \Gamma_k \right\} d\tau = 0.$$

In order that this relation applies to any volume V within the solid C , we must have

$$\frac{1}{2} \varepsilon_{ijk} \left[\frac{\partial}{\partial x_l} (x_i T_{lj} - x_j T_{li}) \right] + \Gamma_k = 0$$

or

$$\frac{1}{2} \varepsilon_{ijk} \left[x_i \left(\frac{\partial T_{lj}}{\partial x_l} + F_j \rho \right) - x_j \left(\frac{\partial T_{li}}{\partial x_l} + F_i \rho \right) + T_{ij} - T_{ji} \right] + \Gamma_k = 0.$$

Taking into account the continuity condition (1.3.2.5), this equation reduces to

$$\frac{1}{2} \varepsilon_{ijk} [T_{ij} - T_{ji}] + \Gamma_k = 0.$$

A volume couple can occur for instance in the case of a magnetic or an electric field acting on a body that locally possesses magnetic or electric moments. In general, apart from very rare cases, one can ignore these volume couples. One can then deduce that the stress tensor is symmetrical:

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$$T_{ij} - T_{ji} = 0.$$

This result can be recovered by applying the relation (1.3.2.2) to a small volume in the form of an elementary parallelepiped, thus illustrating the demonstration using Green's theorem but giving insight into the action of the constraints. Consider a rectangular parallelepiped, of sides $2\Delta x_1$, $2\Delta x_2$ and $2\Delta x_3$, with centre P at the origin of an orthonormal system whose axes Px_1 , Px_2 and Px_3 are normal to the sides of the parallelepiped (Fig. 1.3.2.4). In order that the resultant moment with respect to a point be zero, it is necessary that the resultant moments with respect to three axes concurrent in this point are zero. Let us write for instance that the resultant moment with respect to the axis Px_3 is zero. We note that the constraints applied to the faces perpendicular to Px_3 do not give rise to a moment and neither do the components T_{11} , T_{13} , T_{22} and T_{23} of the constraints applied to the faces normal to Px_1 and Px_2 (Fig. 1.3.2.4). The components T_{12} and T_{21} alone have a nonzero moment.

For face 1, the constraint is $T_{12} + (\partial T_{12}/\partial x_1)\Delta x_1$ if T_{12} is the magnitude of the constraint at P . The force applied at face 1 is

$$\left[T_{12} + \frac{\partial T_{12}}{\partial x_1} \Delta x_1 \right] 4\Delta x_2 \Delta x_3$$

and its moment is

$$\left[T_{12} + \frac{\partial T_{12}}{\partial x_1} \Delta x_1 \right] 4\Delta x_2 \Delta x_3 \Delta x_1.$$

Similarly, the moments of the force on the other faces are

$$\text{Face } 1' : - \left[T_{12} + \frac{\partial T_{12}}{\partial x_1} (-\Delta x_1) \right] 4\Delta x_2 \Delta x_3 (-\Delta x_1);$$

$$\text{Face } 2 : \left[T_{21} + \frac{\partial T_{21}}{\partial x_2} \Delta x_2 \right] 4\Delta x_1 \Delta x_3 \Delta x_2;$$

$$\text{Face } 2' : - \left[T_{21} + \frac{\partial T_{21}}{\partial x_2} (-\Delta x_2) \right] 4\Delta x_1 \Delta x_3 (-\Delta x_2).$$

Noting further that the moments applied to the faces 1 and 1' are of the same sense, and that those applied to faces 2 and 2' are of the opposite sense, we can state that the resultant moment is

$$[T_{12} - T_{21}] 8\Delta x_1 \Delta x_2 \Delta x_3 = [T_{12} - T_{21}] \Delta \tau,$$

where $8\Delta x_1 \Delta x_2 \Delta x_3 = \Delta \tau$ is the volume of the small parallelepiped. The resultant moment per unit volume, taking into account the couples in volume, is therefore

$$T_{12} - T_{21} + \Gamma_3.$$

It must equal zero and the relation given above is thus recovered.

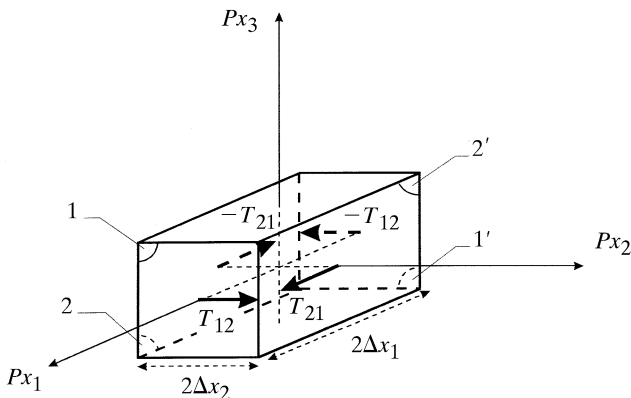


Fig. 1.3.2.4. Symmetry of the stress tensor: the moments of the couples applied to a parallelepiped compensate each other.

1.3.2.5. Voigt's notation – interpretation of the components of the stress tensor

1.3.2.5.1. Voigt's notation, reduced form of the stress tensor

We shall use frequently the notation due to Voigt (1910) in order to express the components of the stress tensor:

$$\begin{aligned} T_1 &= T_{11}; & T_2 &= T_{22}; & T_3 &= T_{33}; \\ T_4 &= T_{23} = T_{32}; & T_5 &= T_{31} = T_{13}; & T_6 &= T_{12} = T_{21}. \end{aligned}$$

It should be noted that the conventions are different for the Voigt matrices associated with the stress tensor and with the strain tensor (Section 1.3.1.3.1).

The Voigt matrix associated with the stress tensor is therefore of the form

$$\begin{pmatrix} T_1 & T_6 & T_5 \\ T_6 & T_2 & T_4 \\ T_5 & T_4 & T_3 \end{pmatrix}.$$

1.3.2.5.2. Interpretation of the components of the stress tensor – special forms of the stress tensor

(i) *Uniaxial stress*: let us consider a solid shaped like a parallelepiped whose faces are normal to three orthonormal axes (Fig. 1.3.2.5). The terms of the main diagonal of the stress tensor correspond to uniaxial stresses on these faces. If there is a single uniaxial stress, the tensor is of the form

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & T_3 \end{pmatrix}.$$

The solid is submitted to two equal and opposite forces, $T_{33}S_3$ and $-T_{33}S_3$, where S_3 is the area of the face of the parallelepiped that is normal to the Ox_3 axis (Fig. 1.3.2.5a). The convention used in general is that there is a uniaxial *compression* if $T_3 \leq 0$ and a uniaxial *traction* if $T_3 \geq 0$, but the opposite sign convention is sometimes used, for instance in applications such as piezoelectricity or photoelasticity.

(ii) *Pure shear stress*: the tensor reduces to two equal uniaxial constraints of opposite signs (Fig. 1.3.2.5b):

$$\begin{pmatrix} T_1 & 0 & 0 \\ 0 & -T_1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

(iii) *Hydrostatic pressure*: the tensor reduces to three equal uniaxial stresses of the same sign (it is spherical):

$$\begin{pmatrix} -p & 0 & 0 \\ 0 & -p & 0 \\ 0 & 0 & -p \end{pmatrix},$$

where p is a positive scalar.

(iv) *Simple shear stress*: the tensor reduces to two equal nondiagonal terms (Fig. 1.3.2.5c), for instance $T_{12} = T_{21} = T_6$. T_{12} represents the component parallel to Ox_2 of the stress applied to face 1 and T_{21} represents the component parallel to Ox_1 of the stress applied to face 2. These two stresses generate opposite couples that compensate each other. It is important to note that it is impossible to have one nondiagonal term only: its effect would be a couple of rotation of the solid and not a deformation.

1.3.2.6. Boundary conditions

If the surface of the solid C is free from all exterior action and is in equilibrium, the stress field T_{ij} inside C is zero at the surface. If C is subjected from the outside to a distribution of stresses T_n

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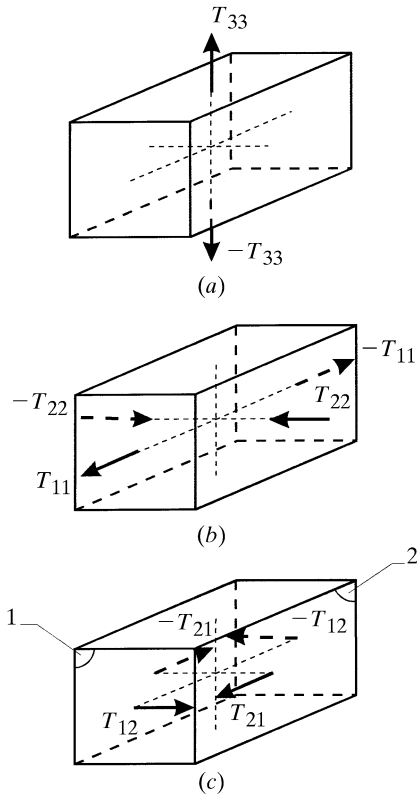


Fig. 1.3.2.5. Special forms of the stress tensor. (a) Uniaxial stress: the stress tensor has only one component, T_{33} ; (b) pure shear stress: $T_{22} = -T_{11}$; (c) simple shear stress: $T_{21} = T_{12}$.

(apart from the volume forces mentioned earlier), the stress field inside the solid is such that at each point of the surface

$$T_{nj} = T_{ij}\alpha_i,$$

where the α_j 's are the direction cosines of the normal to the surface at the point under consideration.

1.3.2.7. Local properties of the stress tensor

(i) *Normal stress and shearing stress*: let us consider a surface area element $d\sigma$ within the solid, the normal \mathbf{n} to this element and the stress \mathbf{T}_n that is applied to it (Fig. 1.3.2.6).

The *normal stress*, ν , is, by definition, the component of \mathbf{T}_n on \mathbf{n} ,

$$\nu = \mathbf{n}(\mathbf{T}_n \cdot \mathbf{n})$$

and the *shearing stress*, τ , is the projection of \mathbf{T}_n on the surface area element,

$$\tau = \mathbf{n} \wedge (\mathbf{T}_n \wedge \mathbf{n}) = \mathbf{T}_n - \nu \mathbf{n}.$$

(ii) *The stress quadric*: let us consider the bilinear form attached to the stress tensor:

$$f(\mathbf{y}) = T_{ij}y_i y_j.$$

The quadric represented by

$$f(\mathbf{y}) = \varepsilon$$

is called the stress quadric, where $\varepsilon = \pm 1$. It may be an ellipsoid or a hyperboloid. Referred to the principal axes, and using Voigt's notation, its equation is

$$y_i^2 T_i = \varepsilon.$$

To every direction \mathbf{n} of the medium, let us associate the radius vector \mathbf{y} of the quadric (Fig. 1.3.2.7) through the relation

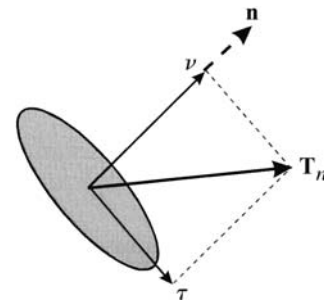


Fig. 1.3.2.6. Normal (ν) and shearing (τ) stress.

$$\mathbf{n} = k\mathbf{y}.$$

The stress applied to a small surface element $d\sigma$ normal to \mathbf{n} , \mathbf{T}_n , is

$$\mathbf{T}_n = k\nabla(f)$$

and the normal stress, ν , is

$$\nu = \alpha_i T_i = 1/y^2,$$

where the α_i 's are the direction cosines of \mathbf{n} .

(iii) *Principal normal stresses*: the stress tensor is symmetrical and has therefore real eigenvectors. If we represent the tensor with reference to a system of axes parallel to its eigenvectors, it is put in the form

$$\begin{pmatrix} T_1 & 0 & 0 \\ 0 & T_2 & 0 \\ 0 & 0 & T_3 \end{pmatrix}.$$

T_1 , T_2 and T_3 are the principal normal stresses. The mean normal stress, T , is defined by the relation

$$T = (T_1 + T_2 + T_3)/3$$

and is an invariant of the stress tensor.

1.3.2.8. Energy density in a deformed medium

Consider a medium that is subjected to a stress field T_{ij} . It has sustained a deformation indicated by the deformation tensor S . During this deformation, the forces of contact have performed work and the medium has accumulated a certain elastic energy W . The knowledge of the energy density thus acquired is useful for studying the properties of the elastic constants. Let the medium deform from the deformation S_{ij} to the deformation $S_{ij} + \delta S_{ij}$ under the influence of the stress field and let us evaluate the work of each component of the effort. Consider a small elementary rectangular parallelepiped of sides $2\Delta x_1$, $2\Delta x_2$, $2\Delta x_3$ (Fig. 1.3.2.8). We shall limit our calculation to the components T_{11} and T_{12} , which are applied to the faces 1 and 1', respectively.

In the deformation δS , the point P goes to the point P' , defined by

$$\mathbf{PP}' = \mathbf{u}(\mathbf{r}).$$

A neighbouring point Q goes to Q' such that (Fig. 1.3.1.1)

$$\mathbf{PQ} = \Delta \mathbf{r}; \quad \mathbf{P}'Q' = \delta \mathbf{r}'.$$

The coordinates of $\delta \mathbf{r}'$ are given by

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

Of sole importance is the relative displacement of Q with respect to P and the displacement that must be taken into account in calculating the forces applied at Q . The coordinates of the relative displacement are

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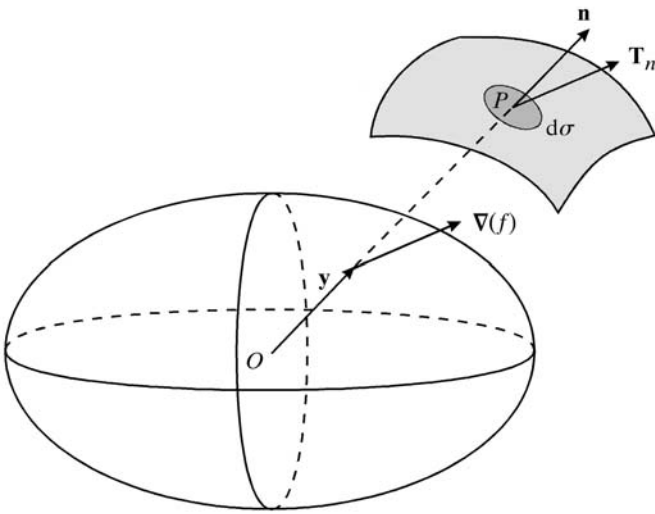


Fig. 1.3.2.7. The stress quadric: application to the determination of the stress applied to a surface element. The surface of the medium is shaded in light grey and a small surface element, $d\sigma$, is shaded in medium grey. The stress at P is proportional to $\nabla(f)$ at the intersection of \mathbf{OP}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

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

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 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*:

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

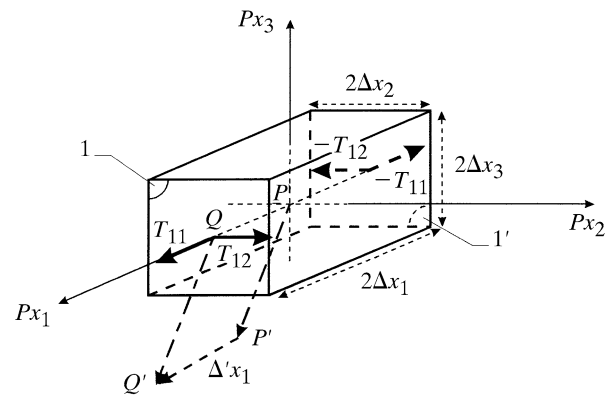


Fig. 1.3.2.8. Determination of the energy density in a deformed medium. \mathbf{PP}' represents the displacement of the small parallelepiped during the deformation. The thick arrows represent the forces applied to the faces 1 and $1'$.

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

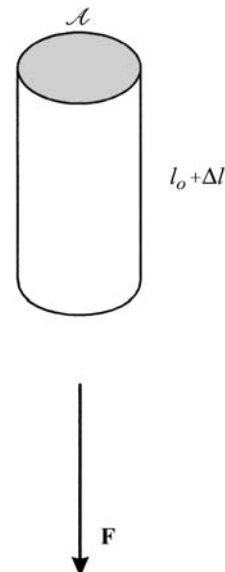


Fig. 1.3.3.1. Bar loaded in pure tension.

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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.

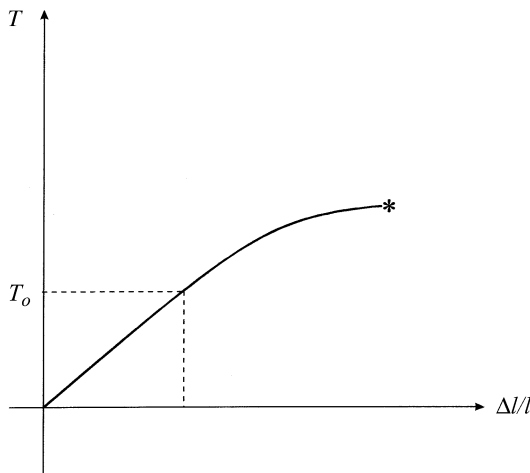


Fig. 1.3.3.2. Schematic stress-strain curve. T : stress; T_0 : elastic limit; $\Delta l/l$: elongation; the asterisk symbolizes the rupture.

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 1×9 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

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

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 6×6 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 relations*: in 1828, the French physicist A.-L. Cauchy expressed the strain energy of a discrete-particle structure when its potential energy depends only on attractive and repulsive cohesive forces between pairs of material points (the so-called central or point-to-point force law). These forces act along the line joining the points and depend on the distances between these points. It can be shown that, if in addition every atom is situated at a centre of symmetry, the elastic constants are totally symmetric in their four indices. Thus,

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

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

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

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

These are known as the Cauchy relations. The further symmetry that they imply reduces the maximum number of independent constants from 21 to 15. In the spherical system (Section 1.1.4.10.6.8), this number is reduced to 1 ($c_{11} = 3c_{12}$). Poisson's ratio, $\nu = -s_{12}/s_{11}$, defined in Section 1.3.3.4.3, is then equal to 0.25, taking into account the relations between s_{11}, s_{12} and c_{11}, c_{12} given in Section 1.3.3.2.3. In practice, Table 1.3.3.2 shows that in real crystals ν is never equal to 0.25, and that Cauchy relations do not apply.

The extent to which Cauchy 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 $c_{12} = c_{66}$, or $\nu \simeq 0.25$, 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.

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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 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.

Table 1.3.3.2. Elastic compliances of some cubic materials in (GPa)⁻¹ (after Every & McCurdy, 1992)

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	2.63	-0.74	9.20	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	7.73	-2.15	12.20	0.279	0.636
W	2.45	-0.69	6.24	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	22.9	-4.8	78.3	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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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

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

The matrix coefficients A_{1i} 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, $\bar{3}$):

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

(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 aluminium (Fig. 1.3.3.4a), tungsten (Fig. 1.3.3.4b) and sodium chloride (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, $3m$). 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 aluminium, smaller than 1 for sodium chloride 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

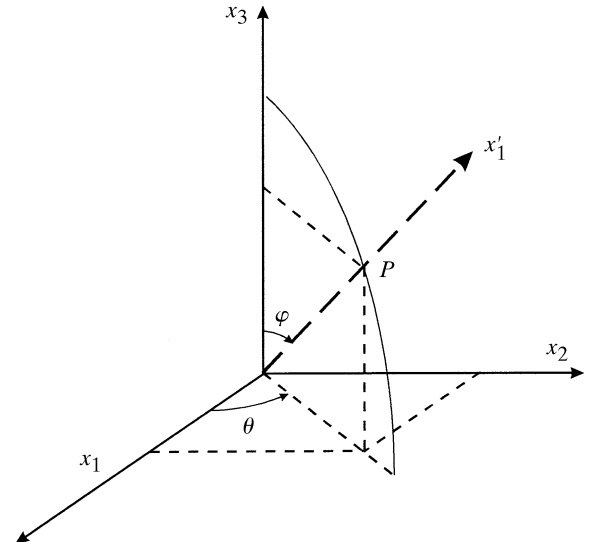


Fig. 1.3.3.3. Spherical coordinates.

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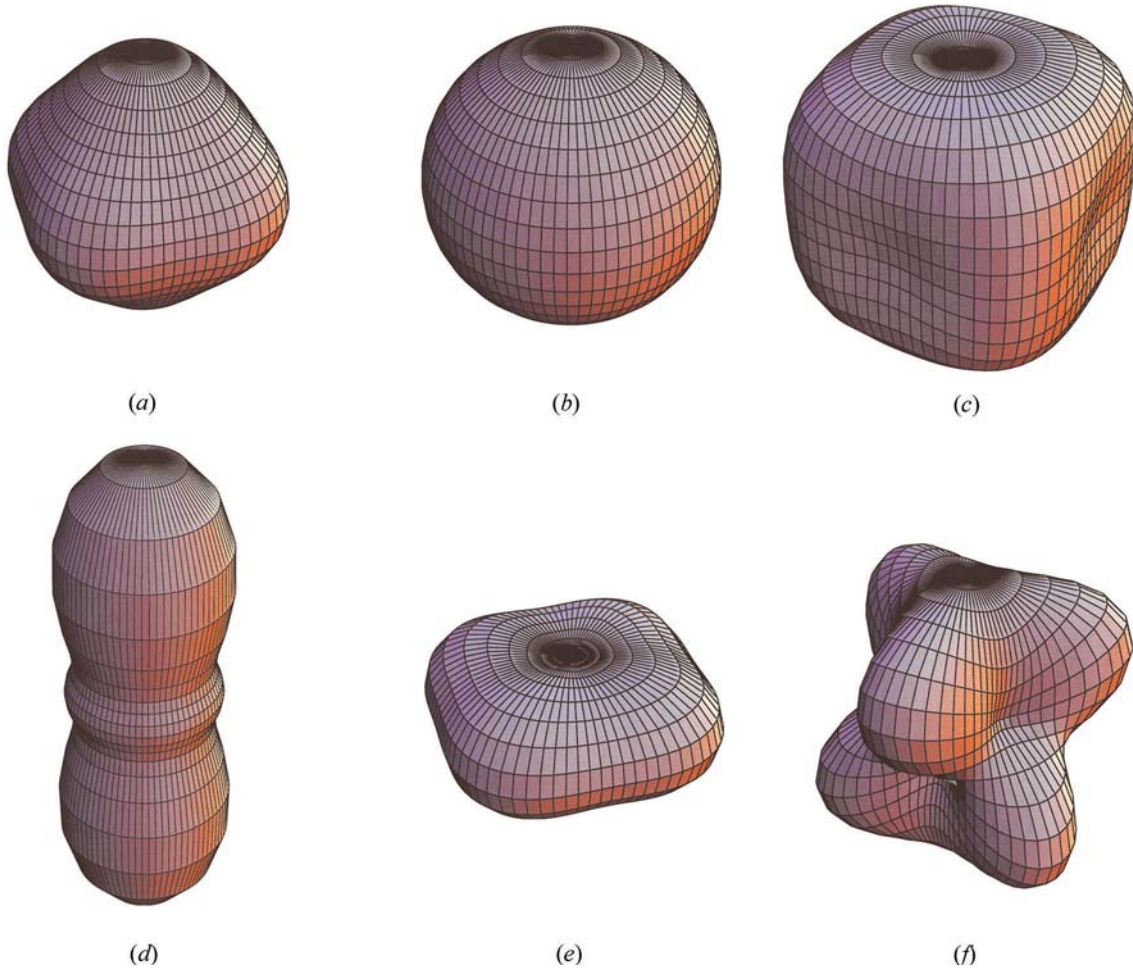


Fig. 1.3.3.4. Representation surface of the inverse of Young's modulus. (a) Al, cubic, anisotropy factor > 1 ; (b) W, cubic, anisotropy factor $= 1$; (c) NaCl, cubic, anisotropy factor < 1 ; (d) Zn, hexagonal; (e) Sn, tetragonal; (f) calcite, trigonal.

$$\begin{aligned}
 T_1 &= c_{11}S_1 + c_{12}(S_2 + S_3) & T_1 &= 2\mu S_1 + \lambda(S_1 + S_2 + S_3) \\
 T_2 &= c_{12}S_1 + c_{11}S_2 + c_{12}S_3 & T_2 &= 2\mu S_2 + \lambda(S_1 + S_2 + S_3) \\
 T_3 &= c_{12}(S_1 + S_2) + c_{11}S_3 & T_3 &= 2\mu S_3 + \lambda(S_1 + S_2 + S_3).
 \end{aligned} \tag{1.3.3.16}$$

These relations can equally well be written in the symmetrical form

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

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:

Coefficient	In terms of μ and λ	In terms of μ and ν	In terms of c_{11} and c_{12}
c_{11}	$2\mu + \lambda$	$2\mu(1 - \nu)/(1 - 2\nu)$	c_{11}
c_{12}	λ	$2\mu\nu/(1 - 2\nu)$	c_{12}
$c_{44} = 1/s_{44}$	μ	μ	$(c_{11} - c_{12})/2$
$E = 1/s_{11}$	$\mu(2\mu + 3\lambda)/(\mu + \lambda)$	$2\mu(1 + \nu)$	See Section 1.3.3.2.3
s_{12}	$-\lambda/[2\mu(2\mu + 3\lambda)]$	$-\nu/[2\mu(1 + \nu)]$	See Section 1.3.3.2.3
κ	$3/(2\mu + 3\lambda)$	$3(1 - 2\nu)/[2\mu(1 + \nu)]$	$3/(c_{11} + 2c_{12})$
$\nu = -s_{12}/s_{11}$	$\lambda/[2(2\mu + 3\lambda)]$	ν	$c_{11}/(c_{11} + c_{12})$

Two coefficients suffice to define the elastic properties of an isotropic material, s_{11} and s_{12} , c_{11} and c_{12} , μ and λ , μ and ν , 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, $\mathbf{u}(\mathbf{r})$:

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

$$c_{ijkl} \frac{\partial^2 u_k}{\partial x_i \partial x_j} = \rho \frac{\partial^2 x_i}{\partial t^2}. \quad (1.3.4.3)$$

In an isotropic orthonormal medium, this equation, projected on the axis Ox_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.

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

1.3.4. Propagation of elastic waves in continuous media – dynamic elasticity

1.3.4.1. Introduction

The elastic properties of materials have been considered in the preceding section in the static state and the elastic constants have been defined in terms of the response of the material to particular static forces. It is effectively the way the elastic constants have been measured in the past, although the measurements could not be very precise. A way of proceeding frequently used now is to excite a mechanical wave in the crystal and measure its propagation velocity or the wavelength associated with a particular frequency. One method consists in sending a train of ultrasonic waves through the crystal; one uses a pulse generator and a piezoelectric transducer glued to the crystal. The elapsed time between the emission of the train of waves and its reception after reflection from the rear face of the sample is then measured. Another method involves producing a system of standing waves after reflection at the inner surface of the crystal and determining the set of resonance frequencies. The experimental techniques will be described in Section 1.3.4.6.

The purpose of the next sections is to establish relations between the wavelength – or the velocity of propagation – and the elastic constants.

1.3.4.2. Equation of propagation of a wave in a material

Consider the propagation of a wave in a continuous medium. The elongation of each point will be of the form

$$\mathbf{u} = \mathbf{u}_0 \exp(2\pi i \nu t) \exp(-2\pi i \mathbf{q} \cdot \mathbf{r}), \quad (1.3.4.1)$$

where ν is the frequency and \mathbf{q} is the wavevector. The velocity of propagation of the wave is

$$V = \nu/q. \quad (1.3.4.2)$$

We saw in Section 1.3.3.6 that the equilibrium condition is

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

Here the only volume forces that we must consider are the inertial forces:

The position vector of the point under consideration is of the form

$$\mathbf{r} = \mathbf{r}_0 + \mathbf{u},$$

where only \mathbf{u} depends on the time and \mathbf{r}_0 defines the mean position. Equation (1.3.4.3) is written therefore

$$c_{ijkl} \frac{\partial^2 u_k}{\partial x_i \partial x_j} = \rho \frac{\partial^2 u_i}{\partial t^2}. \quad (1.3.4.4)$$

Replacing \mathbf{u} by its value in (1.3.4.1), dividing by $-4\pi^2$ and using orthonormal coordinates, we get

$$c_{ijkl} u_k q_j q_l = \rho v^2 u_i. \quad (1.3.4.5)$$

It can be seen that, for a given wavevector, ρv^2 appears as an eigenvalue of the matrix $c_{ijkl} u_k q_j q_l$ of which the vibration vector \mathbf{u} is an eigenvector. This matrix is called the dynamical matrix, or *Christoffel matrix*. In order that the system (1.3.4.5) has a solution other than a trivial one, it is necessary that the associated determinant be equal to zero. It is called the Christoffel determinant and it plays a fundamental role in the study of the propagation of elastic waves in crystals.

Let $\alpha_1, \alpha_2, \alpha_3$ be the direction cosines of the wavevector \mathbf{q} . The components of the wavevector are

$$q_i = q \alpha_i.$$

With this relation and (1.3.4.2), the system (1.3.4.5) becomes

$$c_{ijkl} u_k \alpha_j \alpha_l = \rho v^2 u_i. \quad (1.3.4.6)$$

Putting

$$\Gamma_{ik} = c_{ijkl} \alpha_j \alpha_l \quad (1.3.4.7)$$

in (1.3.4.6), the condition that the Christoffel determinant is zero can be written

$$\Delta(\Gamma_{ik} - \rho v^2 \delta_{ik}) = 0. \quad (1.3.4.8)$$

On account of the intrinsic symmetry of the tensor of elastic stiffnesses, the matrix Γ_{ik} is symmetrical.

If we introduce into expression (1.3.4.7) the elastic stiffnesses with two indices [equation (1.3.3.6)], we find, for instance, for Γ_{11} and Γ_{12}

$$\Gamma_{11} = c_{11}(\alpha_1)^2 + c_{66}(\alpha_2)^2 + c_{55}(\alpha_3)^2 + 2c_{16}\alpha_1\alpha_2$$

$$+ 2c_{15}\alpha_1\alpha_3 + 2c_{56}\alpha_2\alpha_3$$

$$\Gamma_{12} = c_{16}(\alpha_1)^2 + c_{26}(\alpha_2)^2 + c_{45}(\alpha_3)^2 + (c_{12} + c_{66})\alpha_1\alpha_2$$

$$+ (c_{14} + c_{56})\alpha_1\alpha_3 + (c_{46} + c_{25})\alpha_2\alpha_3.$$

The expression for the effective value, c_{ijkl}^e , of the 'stiffened' elastic stiffness in the case of piezoelectric crystals is given in Section 2.4.2.2.

1.3.4.3. Dynamic elastic stiffnesses

Equation (1.3.4.7) may be written

$$\Gamma_{ik} = \sum_{j \neq l} [c_{ijkl} + c_{ilkj}] \alpha_j \alpha_l.$$

This shows that in a dynamic process only the sums $[c_{ijkl} + c_{ilkj}]$ can be measured and not c_{ijkl} and c_{ilkj} separately. On the contrary, c_{ijij} can be measured directly. In the cubic system therefore, for instance, c_{1122} is determined from the measurement

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of $[c_{1122} + c_{1221}]$ on the one hand and from that of c_{1221} on the other hand.

1.3.4.4. Polarization of the elastic waves

The Christoffel determinant has three roots and the Christoffel matrix, being Hermitian with real coefficients, has three real eigenvalues and three orthogonal eigenvectors. The wavevector \mathbf{q} , therefore, encompasses three waves with vibration vectors \mathbf{u}_1 , \mathbf{u}_2 , \mathbf{u}_3 which are perpendicular to one another. In the general case, there is no particular angular relationship between the vibration vectors (or polarization vectors). However, if the latter are parallel to certain symmetry directions in the crystal, one of the vibration vectors is along this direction. The corresponding wave is called longitudinal. The two other waves have their polarization direction perpendicular to the wavevector and are thus transverse. If one of the polarization vectors is almost parallel to the wavevector, which often happens, then one speaks of the vibration as being quasi-longitudinal.

1.3.4.5. Relation between velocity of propagation and elastic stiffnesses

We shall limit ourselves to cubic, hexagonal and tetragonal crystals and consider particular cases.

1.3.4.5.1. Cubic crystals

(i) *The wavevector is parallel to [100].* The Christoffel determinant reduces to

$$\begin{pmatrix} c_{11} - \rho v^2 & 0 & 0 \\ 0 & c_{44} - \rho v^2 & 0 \\ 0 & 0 & c_{44} - \rho v^2 \end{pmatrix} = 0.$$

The three solutions are given in Table 1.3.4.1. These results are valid for a wave propagating in any direction in an isotropic medium.

(ii) *The wavevector is parallel to [110].* The direction cosines of the wavevector are $1/\sqrt{2}$, $1/\sqrt{2}$, 0. The Christoffel determinant assumes the form

$$\begin{pmatrix} \frac{1}{2}(c_{11} + c_{44}) - \rho v^2 & \frac{1}{2}(c_{12} + c_{44}) & 0 \\ \frac{1}{2}(c_{12} + c_{44}) & \frac{1}{2}(c_{11} + c_{44}) - \rho v^2 & 0 \\ 0 & 0 & c_{44} - \rho v^2 \end{pmatrix} = 0.$$

The three solutions are given in Table 1.3.4.2.

(iii) *The wavevector is parallel to [111].* The Christoffel determinant assumes the form

$$\begin{pmatrix} c_{11} + 2c_{44} - \rho v^2 & c_{12} + c_{44} & c_{12} + c_{44} \\ c_{12} + c_{44} & c_{11} + 2c_{44} - \rho v^2 & c_{12} + c_{44} \\ c_{12} + c_{44} & c_{12} + c_{44} & c_{44} - \rho v^2 \end{pmatrix} = 0.$$

The solutions are given in Table 1.3.4.3.

1.3.4.5.2. Hexagonal crystals

In hexagonal crystals, there are five independent elastic stiffnesses, c_{11} , c_{33} , c_{12} , c_{13} , c_{44} and $c_{66} = (c_{11} - c_{12})/2$ (Section 1.1.4.10.4).

(i) *The wavevector is parallel to [001].* The Christoffel determinant reduces to

$$\begin{pmatrix} c_{44} - \rho v^2 & 0 & 0 \\ 0 & c_{44} - \rho v^2 & 0 \\ 0 & 0 & c_{33} - \rho v^2 \end{pmatrix} = 0.$$

The solutions are given in Table 1.3.4.4.

(ii) *The wavevector is parallel to [100].* The Christoffel determinant readily reduces to

$$\begin{pmatrix} c_{11} - \rho v^2 & 0 & 0 \\ 0 & c_{66} - \rho v^2 & 0 \\ 0 & 0 & c_{44} - \rho v^2 \end{pmatrix} = 0.$$

The three solutions are given in Table 1.3.4.5.

1.3.4.5.3. Tetragonal crystals (classes $4mm$, $\bar{4}2m$, $4/mmm$)

In tetragonal crystals, there are six independent elastic stiffnesses, c_{11} , c_{33} , c_{12} , c_{13} , c_{44} and c_{66} (Section 1.1.4.10.4).

(i) *The wavevector is parallel to [001].* The Christoffel determinant reduces to

Table 1.3.4.1. Velocity of propagation when the wavevector is parallel to [100] (cubic crystals)

Velocity of propagation	Polarization vector	Nature of the wave
$v_{\parallel} = \sqrt{c_{11}/\rho}$	[100]	Longitudinal
$v_{\perp} = \sqrt{c_{44}/\rho}$	[010]	Transverse
$v_{\perp} = \sqrt{c_{44}/\rho}$	Any vector normal to [100]	Transverse

Table 1.3.4.2. Velocity of propagation when the wavevector is parallel to [110] (cubic crystals)

Velocity of propagation	Polarization vector	Nature of the wave
$v_{\parallel} = \sqrt{[c_{44} + \frac{1}{2}(c_{11} + c_{12})]/\rho}$	[110]	Longitudinal
$v_{\perp} = \sqrt{\frac{1}{2}(c_{11} - c_{12})/\rho}$	[$\bar{1}10$]	Transverse
$v_{\perp} = \sqrt{c_{44}/\rho}$	[001]	Transverse

Table 1.3.4.3. Velocity of propagation when the wavevector is parallel to [111] (cubic crystals)

Velocity of propagation	Polarization vector	Nature of the wave
$v_{\parallel} = \sqrt{(c_{11} + 2c_{12} + 4c_{44})/3\rho}$	[111]	Longitudinal
$v_{\perp} = \sqrt{(c_{11} - c_{12} + c_{44})/3\rho}$	Any vector normal to [111]	Transverse

Table 1.3.4.4. Velocity of propagation when the wavevector is parallel to [001] (hexagonal crystals)

Velocity of propagation	Polarization vector	Nature of the wave
$v_{\parallel} = \sqrt{c_{33}/\rho}$	[100]	Longitudinal
$v_{\perp} = \sqrt{c_{44}/\rho}$	Any vector normal to [001]	Transverse

Table 1.3.4.5. Velocity of propagation when the wavevector is parallel to [100] (hexagonal crystals)

Velocity of propagation	Polarization vector	Nature of the wave
$v_{\parallel} = \sqrt{c_{11}/\rho}$	[100]	Longitudinal
$v_{\perp} = \sqrt{c_{66}/\rho}$	[010]	Transverse
$v_{\perp} = \sqrt{c_{44}/\rho}$	[001]	Transverse

Table 1.3.4.6. Velocity of propagation when the wavevector is parallel to [001] (tetragonal crystals)

Velocity of propagation	Polarization vector	Nature of the wave
$v_{\parallel} = \sqrt{c_{33}/\rho}$	[100]	Longitudinal
$v_{\perp} = \sqrt{c_{44}/\rho}$	[010]	Transverse
$v_{\perp} = \sqrt{c_{44}/\rho}$	[001]	Transverse

Table 1.3.4.7. Velocity of propagation when the wavevector is parallel to [100] (tetragonal crystals)

Velocity of propagation	Polarization vector	Nature of the wave
$v_{\parallel} = \sqrt{c_{11}/\rho}$	[100]	Longitudinal
$v_{\perp} = \sqrt{c_{66}/\rho}$	[010]	Transverse
$v_{\perp} = \sqrt{c_{44}/\rho}$	[001]	Transverse

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$$\begin{pmatrix} c_{44} - \rho v^2 & 0 & 0 \\ 0 & c_{44} - \rho v^2 & 0 \\ 0 & 0 & c_{33} - \rho v^2 \end{pmatrix} = 0.$$

The three solutions are given in Table 1.3.4.6.

(ii) *The wavevector is parallel to [100]*. The Christoffel determinant reduces to

$$\begin{pmatrix} c_{11} - \rho v^2 & 0 & 0 \\ 0 & c_{66} - \rho v^2 & 0 \\ 0 & 0 & c_{44} - \rho v^2 \end{pmatrix} = 0.$$

The three solutions are given in Table 1.3.4.7.

1.3.4.6. Experimental determination of elastic constants

1.3.4.6.1. Introduction

As mentioned in Section 1.3.4.1, the elastic constants of a material can be obtained by the elastic response of the material to particular static forces; however, such measurements are not precise and the most often used approach nowadays consists of determining the velocity of ultrasonic waves propagating along different directions of the crystal and calculating the elastic constants from the Christoffel determinants (1.3.4.8). The experimental values are often accurate enough to justify the distinction between static and dynamic values of the elastic constants and between phase and group velocities, and the careful consideration of the frequency range of the experiments.

(i) *Static and dynamic elastic constants*. When one measures the elastic response of a material to external static forces, work is done and heat is produced. In general, the external forces are applied slowly (quasi-elastic processes) and the solid body remains in thermal equilibrium with its surroundings, which can be considered as a heat reservoir. In this case, the measured elastic constants are isothermal elastic constants as defined in Section 1.1.5.1. On the contrary, when ultrasonic waves propagate in a solid body, the compressed regions are slightly hotter than the expanded regions; the associated temperature gradients give rise to irreversible processes of thermal conduction. However, in the megahertz or higher-frequency ranges, the processes of heat exchange between different regions or between the solid and its surroundings are slow compared with the period of the ultrasonic wave and hence can be considered as isentropic. In this case, the measured velocities are isentropic and the elastic stiffnesses deduced from them are the adiabatic elastic stiffnesses as defined in Section 1.1.5.4. The differences between isothermal and adiabatic elastic stiffnesses can be calculated from equation (1.1.5.2):

$$\begin{aligned} \delta T_{ij} &= (c_{ijkl})^\Theta \delta S_{kl} - \lambda_{ij} \delta \Theta \\ \delta \sigma &= \lambda_{kl} \delta S_{kl} + \frac{\rho C^S}{\Theta} \delta \Theta. \end{aligned}$$

By combining these two equations, it is possible to obtain relations between the isothermal elastic stiffnesses, $(c_{ijkl})^\Theta$, and the adiabatic elastic stiffnesses, $(c_{ijkl})^\sigma$:

$$(c_{ijkl})^\sigma = (c_{ijkl})^\Theta + \frac{\lambda_{ij} \lambda_{kl}}{\rho C^S},$$

where c^S is the specific heat at constant strain.

This relation shows that adiabatic elastic stiffnesses are larger than isothermal elastic stiffnesses, at least for the terms of the main diagonal of the elastic matrix. In general, the differences between isothermal and adiabatic elastic stiffnesses are less than 1%. An exception to this statement concerns the temperature region near the critical temperature T_c where a phase transition occurs.

(ii) *Frequency dependence of the elastic constants*. Dynamic measurements of the elastic constants can be performed at a wide range of ultrasonic frequencies. Currently used techniques for investigating a wide range of frequencies are electronic pulse-echo techniques in the megahertz frequency range and Brillouin scattering in the 10 GHz frequency range. To evaluate the possible differences between dynamic elastic constants determined in different frequency ranges, high-accuracy measurements of the *absolute value* of the elastic constants are required. From optical resonance techniques in the megahertz frequency range and Brillouin scattering in the gigahertz frequency range, it has been shown that the results are the same within 0.1 to 0.2% in the case of simple and stable crystals such as sodium chloride when the ultrasonic waves can be considered as a 'passive probe' (Michard *et al.*, 1971). Larger differences are observed when ultrasonic waves interact with the medium, when they favour or impede structural changes of the material or when they are absorbed for a particular frequency.

(iii) *Phase velocity and group velocity*. When the velocity of ultrasonic waves is frequency dependent (dispersive medium), one has to distinguish phase velocity and group velocity. If a resonance technique is used, the resonance frequencies correspond to phase-matching conditions and the calculation of velocity from the resonance frequencies leads to '*phase velocity*'. If a pulse-echo technique is used, the transit time of an elastic pulse is measured and the interpretation of the measurement is more complex. In this case, Brillouin (1932) has shown that the head and the tail of the pulse travel with the group velocity. Differences of a few per cent can be observed between phase and group velocities in dispersive media.

1.3.4.6.2. Resonance technique

The use of the resonance technique is a well established approach for determining the velocity of sound in a gas by observing nodes and antinodes of a system of standing waves produced in the so-called *Kund tube*. In the case of transparent solids, optical means allow us to visualize the standing waves and to measure the wavelength directly (Zarembowitch, 1965). An easier procedure can be used: let us consider a transparent crystal in the shape of a parallelepiped (Fig. 1.3.4.1). A piezoelectric transducer is glued to the crystal and excited at varying frequencies. If the bonding between the transducer and the crystal is loose enough, the crystal can be considered as free from stress and the sequence of its resonance frequencies is given by

$$v = nV/2l,$$

where n is an integer, V the phase velocity of the wave in the direction orthogonal to the parallel faces and l the distance between these faces.

The looseness of the bonding can be checked by the regularity of the arithmetic ratio, $V/2l$. On account of the elasto-optic coupling, a phase grating is associated with the elastic standing-wave system and a light beam can be diffracted by this grating. The intensity of the diffraction pattern is maximum when resonance occurs. A large number of resonance frequencies can be detected, usually more than 100, sometimes 1000 for non-attenuating materials. Consequently, in favourable cases the absolute value of the ultrasonic velocity can be determined with an uncertainty less than 10^{-3} .

1.3.4.6.3. Pulse-echo techniques

Pulse-echo techniques are valid for transparent and opaque materials. They are currently used for measuring ultrasonic velocities in solids and can be used in very simple as well as in sophisticated versions according to the required precision (McSkimmin, 1964). In the simplest version (Fig. 1.3.4.2), an

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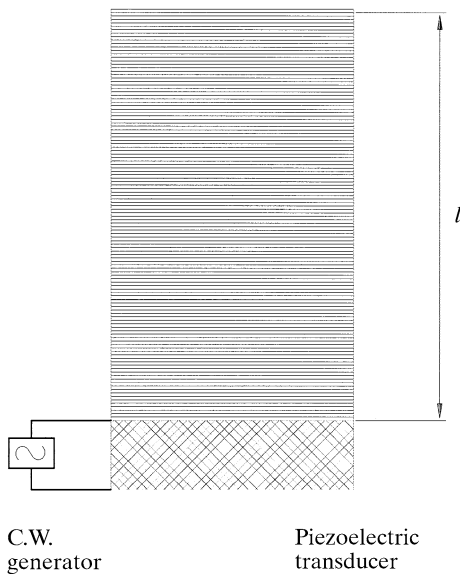


Fig. 1.3.4.1. Resonance technique: standing waves excited in a parallelepiped.

electronic pulse generator excites the mechanical vibrations of a piezo-electric transducer glued to one of two plane-parallel faces of a specimen. An ultrasonic pulse whose duration is of the order of a microsecond is generated and transmitted through the specimen. After reflection at the opposite face, it returns and, when it arrives back at the transducer, it gives rise to an electronic signal, or echo. The whole sequence of such echos is displayed on the screen of an oscilloscope and it is possible to measure from them the time interval for transit. Usually, *X*-cut quartz crystals or ferroelectric ceramics are used to excite longitudinal waves and *Y*-cut quartz is used to excite transverse waves. In many cases, a circulator, or gate, is used to protect the receiver from saturation following the main 'bang'. This method is rough because the beginning and the end of a pulse are not well characterized. Several improvements have therefore been made, mainly based on interferometric techniques (pulse-superposition method, 'sing around' method *etc.*). Nevertheless, if the absolute value of the ultrasonic velocity is not determined with a high accuracy by using pulse-echo techniques, this approach has proved valuable when relative values of ultrasonic velocities are needed, *e.g.* temperature and pressure dependences of ultrasonic velocities.

(i) *Pulse-superposition method.* A piezoelectric transducer initiates ultrasonic pulses in the specimen. These pulses echo back and forth within the specimen. A continuous-wave oscillator

is used to control the pulse repetition rate. When the repetition rate is adjusted so that the initiation of a pulse coincides with the return of the first echo from the preceding pulses, the change in the signal amplitude indicates superposition. The pulse rate is a measure of the travel time within the specimen.

(ii) '*Sing around method*'. The 'sing around' method for measuring the velocity of ultrasonic waves involves the use of two piezoelectric transducers, one at each end of the specimen. One transducer receives an impulse from the electronic generator and converts it into an ultrasonic pulse in the specimen. This pulse, after passing through the specimen, is detected by the receiving transducer. The received pulse triggers the electronic generator to initiate a succeeding pulse. The pulse repetition rate is a very sensitive probe for measuring changes of the ultrasonic velocity in the specimen. Relative variations of 10^{-7} can be measured, such as temperature or stress dependences of the velocity.

1.3.5. Pressure dependence and temperature dependence of the elastic constants

1.3.5.1. Introduction

In a solid, the elastic constants are temperature and pressure dependent. As examples, the *temperature dependence* of the elastic stiffnesses of an aluminium single crystal within its stability domain (the melting point is 933 K) and the *pressure dependence* of the elastic stiffnesses of the ternary compound $KZnF_3$ within its stability domain (the crystal becomes unstable for a hydrostatic pressure of about 20 GPa) are shown in Figs. 1.3.5.1 and 1.3.5.2, respectively.

We can observe the following trends, which are general for stable crystals:

(i) From 0 K to about $\Theta_D/5$, where Θ_D is the Debye temperature, the elastic stiffnesses decrease according to a Θ^4 law. From $\Theta_D/5$ to the beginning of the instability domain, the dependence is linear with Θ . In addition, $(\partial c_{ij}/\partial \Theta)_p = 0$ at 0 K as predicted by the third principle of thermodynamics.

(ii) For stable crystals, the *pressure dependence* of the elastic stiffnesses is linear as long as the applied pressure is small compared to the elastic stiffnesses. As an example, a typical order of magnitude for c_{11} in crystals is about 100 GPa and, within the experimental uncertainty, the pressure dependence of c_{11} does not depart from a linear behaviour up to at least 0.2 GPa.

These observations can be quantitatively justified on the basis of an equation of state of a solid:

$$f(T_{ij}, S_{ij}, X, \Theta) = 0,$$

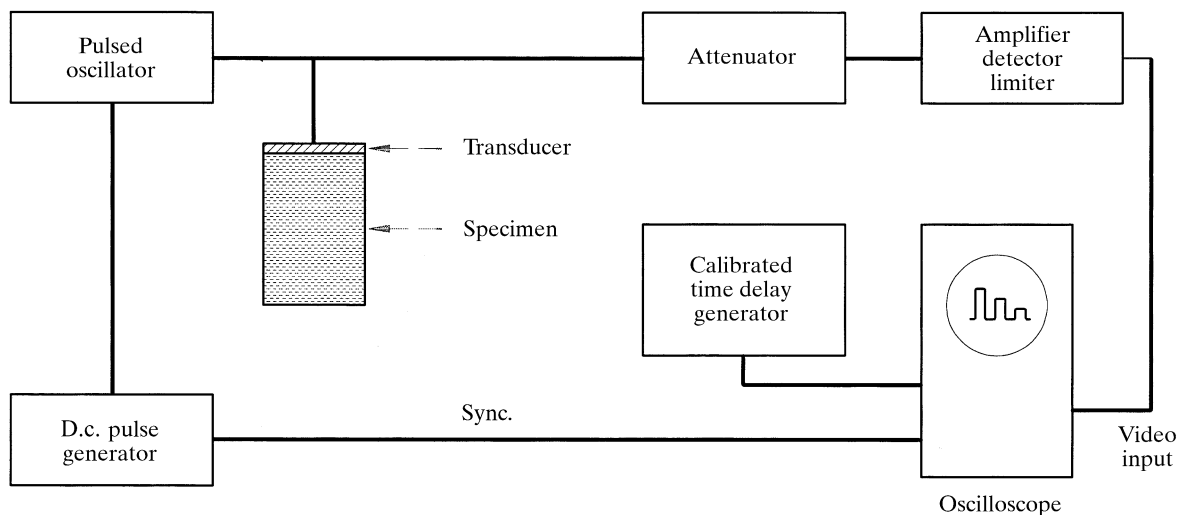


Fig. 1.3.4.2. Block diagram of the pulse-echo technique.

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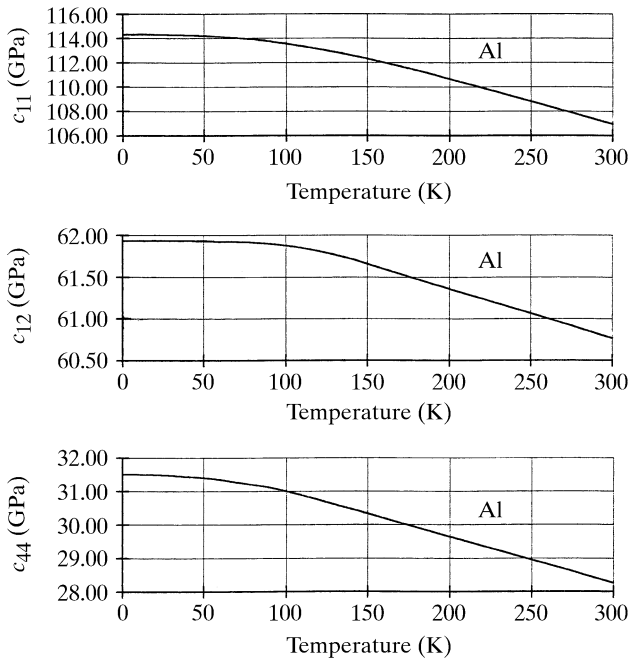


Fig. 1.3.5.1. Temperature dependence of the elastic stiffnesses of an aluminium single crystal (after Every & McCurdy, 1992).

where T_{ij} represents the stress tensor, S_{ij} the strain tensor, X the position of the elementary elements of the solid and Θ the temperature.

Different equations of state of solids have been proposed. They correspond to different degrees of approximation that can only be discussed and understood in a microscopic theory of lattice dynamics. The different steps in the development of lattice dynamics, the Einstein model, the Debye model and the Grüneisen model, will be presented in Section 2.1.2.7. Concerning the temperature and the pressure dependences of the elastic constants, we may notice that rather sophisticated models are needed to describe correctly the general trends mentioned above:

(a) In the *Einstein model*, where the N atoms of a crystal are considered as $3N$ independent harmonic oscillators, the temperature increase affects only the amplitude of the oscillations and not the average positions of the atoms; consequently, this model can explain neither the thermal expansion nor the *temperature dependence* of the elastic constants. In addition, this theory ignores the difference between isothermal and adiabatic elastic constants. Similarly, if the oscillators are harmonic, the stiffness of the ‘springs’ connecting atoms does not depend on the distances between atoms and the model cannot therefore explain the pressure dependence of the elastic constants, which requires anharmonic ‘springs’ or, more accurately, anharmonic potentials.

(b) In the *Debye model*, the $3N$ oscillators are not independent but they are still harmonic. The result is that here again the elastic constants are pressure and temperature independent.

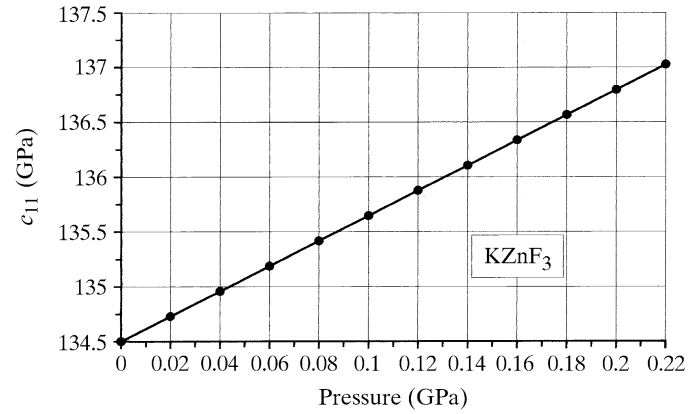


Fig. 1.3.5.2. Pressure dependence of the elastic stiffness c_{11} of a KZnF_3 crystal. Reproduced with permission from *Ultrasonics Symposium Proc. IEEE* (Fischer *et al.*, 1980). Copyright (1980) IEEE.

(c) In the *Grüneisen model*, the frequencies of the oscillators are volume-dependent; this so-called ‘quasiharmonic approximation’ can justify the standard behaviour shown in Figs. 1.3.5.1 and 1.3.5.2.

1.3.5.2. Temperature dependence of the elastic constants

Table 1.3.5.1 gives typical values of $(\partial \ln c_{ij} / \partial \Theta)_p$ for some cubic crystals considered within their stability domain. In column 6, the ‘elastic Debye temperature’ of the crystal, $(\Theta_D)_{el}$, has been calculated according to the formula

$$(\Theta_D)_{el} = hv/k_B(3n/4\pi)^{1/3},$$

where h is the Planck constant, k_B is the Boltzmann constant, v is an average velocity (see for instance De Launay, 1956) and n is the number of atoms per unit volume.

It is interesting to compare $(\Theta_D)_{el}$, the ‘elastic Debye temperature’, with $(\Theta_D)_{cal}$, the ‘calorimetric Debye temperature’. The definition of $(\Theta_D)_{cal}$ will be given in Section 2.1.2.7. It results from the attempt at founding a universal description for the thermal properties of solids when the temperature is expressed as a reduced temperature, $\Theta/(\Theta_D)_{cal}$; $(\Theta_D)_{cal}$ is obtained from calorimetric measurements at low temperature. It is worth noting that accurate values of low-temperature elastic constants and low-temperature calorimetric measurements lead to an excellent agreement between $(\Theta_D)_{el}$ and $(\Theta_D)_{cal}$ [better than 2 or 3 K (De Launay, 1956)]. This agreement demonstrates the validity of the Debye model in the vicinity of 0 K. From Table 1.3.5.1, we can observe that for ionic crystals $(\partial \ln c_{11} / \partial \Theta)_p$ is, in general, greater than $(\partial \ln c_{44} / \partial \Theta)_p$. This remark is not valid for covalent and metallic crystals. Typical orders of magnitude are given in Table 1.3.5.2. These statements concern only general trends valid for stable crystals.

In the case of *temperature-induced phase transitions*, some elastic constants are softened in the vicinity and sometimes far from the critical temperature. As an example, Fig. 1.3.5.3 shows the temperature dependence of c_{44} in RbCdF_3 , CsCdF_3 and TlCdF_3 single crystals. RbCdF_3 and TlCdF_3 undergo structural phase transitions at 124 and 191 K, respectively, while CsCdF_3 remains stable in this temperature range. The softening of c_{44} when the temperature decreases starts more than 100 K before the critical temperature, Θ_c . In contrast, Fig. 1.3.5.4 shows the temperature dependence of c_{11} in KNiF_3 , a crystal that undergoes a para-antiferromagnetic phase transition at 246 K; the coupling between the elastic and the magnetic energy is weak, consequently c_{11} decreases abruptly only a few degrees before the critical temperature. We can generalize this observation and state that the softening of an elastic constant occurs over a large domain of

Table 1.3.5.1. Temperature dependence of the elastic stiffnesses for some cubic crystals

Material	Temperature range (K)	$(\partial \ln c_{11} / \partial \Theta)_p$ (10^{-4} K^{-1})	$(\partial \ln c_{44} / \partial \Theta)_p$ (10^{-4} K^{-1})	$(\partial \ln c_{12} / \partial \Theta)_p$ (10^{-4} K^{-1})	Θ_{el} (K)
Al	80–300	−3.1	−4.45	−1.3	430
Cu	80–300	−2.01	−3.33	−1.24	344
Ag	50–300	−2.3	−4.0	−1.5	226
Pb	100–300	−4.4	−1.5	−2.8	105
Si	80–300	−0.81	−10.6	−1.10	648
Ge	150–1000	−1.2	−1.15	−1.10	374
ZnS	100–300	−1.2	−0.65	−0.8	347
NaCl	100–300	−7.8	−2.2	−4.7	321
KCl	80–300	−8.3	−2.1	−3.6	236
KBr	80–300	−7.6	−2.1	7	172

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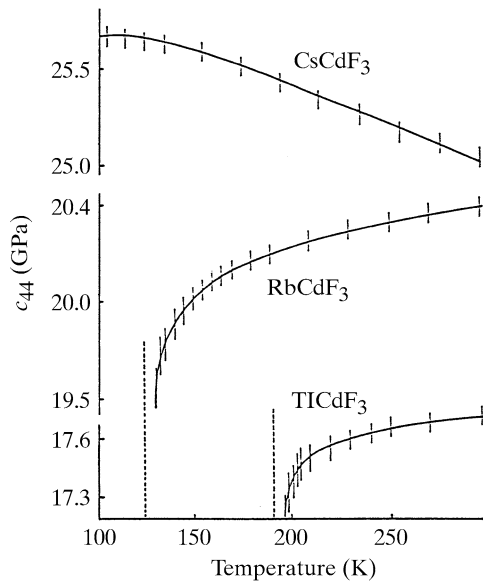


Fig. 1.3.5.3. Temperature dependence of the elastic constant c_{44} in RbCdF_3 , CsCdF_3 and TiCdF_3 crystals; the crystals of RbCdF_3 and TiCdF_3 undergo structural phase transitions (after Rousseau *et al.*, 1975).

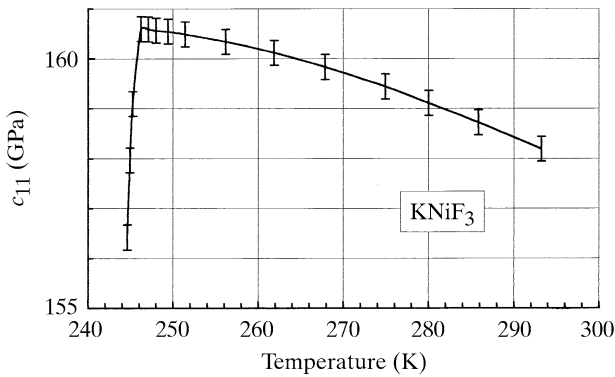


Fig. 1.3.5.4. Temperature dependence of the elastic constant c_{11} in KNiF_3 , which undergoes a para-antiferromagnetic phase transition. Reprinted with permission from *Appl. Phys. Lett.* (Nouet *et al.*, 1972). Copyright (1972) American Institute of Physics.

temperature when this constant is the order parameter or is strongly coupled to the order parameter of the transformation; for instance, in the cooperative Jahn–Teller phase transition in DyVO_4 , $(c_{11} - c_{12})/2$ is the soft acoustic phonon mode leading to the phase transition and this parameter anticipates the phase transition 300 K before it occurs (Fig. 1.3.5.5).

1.3.5.3. Pressure dependence of the elastic constants

As mentioned above, anharmonic potentials are needed to explain the stress dependence of the elastic constants of a crystal. Thus, if the strain-energy density is developed in a polynomial in terms of the strain, only the first and the second elastic constants are used in linear elasticity (harmonic potentials), whereas higher-order elastic constants are also needed for nonlinear elasticity (anharmonic potentials).

Concerning the pressure dependence of the elastic constants (nonlinear elastic effect), considerable attention has been paid to

Table 1.3.5.2. Order of magnitude of the temperature dependence of the elastic stiffnesses for different types of crystals

Type of crystal	$(\partial \ln c_{11} / \partial \Theta)_p$ (K^{-1})	$(\partial \ln c_{44} / \partial \Theta)_p$ (K^{-1})
Ionic	-10^{-3}	-3×10^{-4}
Covalent	-10^{-4}	-8×10^{-5}
Metallic	-2×10^{-4}	-3×10^{-4}

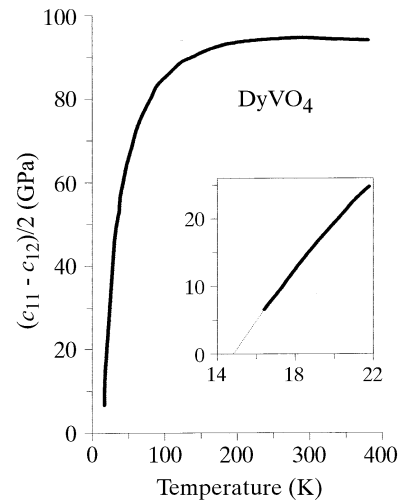


Fig. 1.3.5.5. Temperature dependence of $(c_{11} - c_{12})/2$ in DyVO_4 , which undergoes a cooperative Jahn–Teller phase transition (after Melcher & Scott, 1972).

their experimental determination since they are a unique source of significant information in many fields:

(i) In *geophysics*, a large part of the knowledge we have on the interior of the earth comes from the measurement of the transit time of elastic bursts propagating in the mantle and in the core (in the upper mantle, the average pressure is estimated to be about a few hundred GPa, a value which is comparable to that of the elastic stiffnesses of many materials).

(ii) In *solid-state physics*, the pressure dependence of the elastic constants gives significant indications concerning the stability of crystals. For example, Fig. 1.3.5.2 shows the pressure dependence of the elastic constants of KZnF_3 , a cubic crystal belonging to the perovskite family. As mentioned previously, this crystal is known to be stable over a wide range of temperature and the elastic stiffnesses c_{ij} depend linearly on pressure. It may be noted that, consequently, the third-order elastic constants (TOECs) are constant. On the contrary, we observe in Fig. 1.3.5.6 that the pressure dependence of the elastic constants of TiCdF_3 , a cubic crystal belonging to the same family but which is known to become unstable when the temperature is decreased to 191 K (Fischer, 1982), is nonlinear even at low pressures. In this case, the development of the strain-energy density in terms of strains elastic constant; the contributions of the fourth- and fifth-order elastic constants are not negligible.

(iii) For practical use in the case of technical materials such as concrete or worked metals, the pressure dependence of the elastic moduli is also required for examining the effect of applied stresses or of an applied hydrostatic pressure, and for studying residual stresses resulting from loading (heating) and unloading (cooling) the materials.

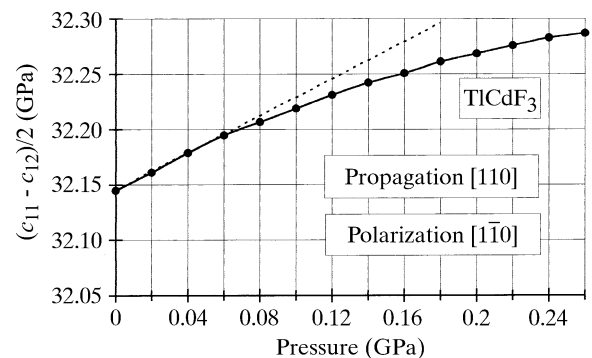


Fig. 1.3.5.6. Pressure dependence of the elastic constants $(c_{11} - c_{12})/2$ in TiCdF_3 . Reproduced with permission from *Ultrasonics Symposium Proc. IEEE* (Fischer *et al.*, 1980). Copyright (1980) IEEE.

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

1.3.6. Nonlinear elasticity

1.3.6.1. Introduction

In a solid body, the relation between the stress tensor T and the strain tensor S is usually described by Hooke's law, which postulates linear relations between the components of T and S (Section 1.3.3.1). Such relations can be summarized by (see equation 1.3.3.2)

$$T_{ij} = c_{ijkl} S_{kl},$$

where the c_{ijkl} 's are the elastic stiffnesses.

For a solid under finite strain conditions, Hooke's law, valid for infinitesimal deformations, does not hold, and the fundamental definitions for stress and strain must be revisited.

1.3.6.2. Lagrangian and Eulerian descriptions

Finite elastic strains may be treated from two different viewpoints using either the *Lagrangian (material)* or the *Eulerian (spatial)* descriptions.

Let us consider a fixed rectangular Cartesian coordinate system with axes x_i ($i = 1, 2, 3$). Any particular position vector \mathbf{r} of components (x_1, x_2, x_3) denotes a point in space. A point that always moves with the material is called a particle or *material point*. Let every particle be identified by its coordinates at some reference time t_0 . These reference coordinates, referred to the same Cartesian system, will be denoted by (a_1, a_2, a_3) and the corresponding position vector \mathbf{a} . A particular vector \mathbf{a} can serve as a name for the particle located at that position at the reference time t_0 .

The vectors \mathbf{r} and \mathbf{a} both specify a position in a fixed Cartesian frame of reference. At any time, we associate each \mathbf{r} with an \mathbf{a} by the rule that \mathbf{r} is the present position vector of the particle initially at \mathbf{a} . This connection between \mathbf{r} and \mathbf{a} is written symbolically as

$$\mathbf{r} = \mathbf{r}(t, \mathbf{a}) \quad \text{or} \quad x_i = x_i(t, a_1, a_2, a_3), \quad (1.3.6.1)$$

where

$$\mathbf{a} = \mathbf{r}(t_0, \mathbf{a}) \quad \text{or} \quad a_i = x_i(t_0, a_1, a_2, a_3). \quad (1.3.6.2)$$

The coordinates a_i that identify the particles are called *material coordinates*. A description that, like (1.3.6.1), uses (t, a_1, a_2, a_3) as independent variables is called a *material* or *Lagrangian* description.

The converse of (1.3.6.1) and (1.3.6.2) may be written

$$\mathbf{a} = \mathbf{a}(t, \mathbf{r}) \quad \text{or} \quad a_i = a_i(t, x_1, x_2, x_3), \quad (1.3.6.3)$$

where

$$\mathbf{r} = \mathbf{a}(t_0, \mathbf{r}) \quad \text{or} \quad x_i = a_i(t_0, x_1, x_2, x_3). \quad (1.3.6.4)$$

A spatial description or *Eulerian* description uses the independent variables (t, x_1, x_2, x_3) , the x_i being called *spatial coordinates*.

Now, for the sake of simplicity, we shall work with the Lagrangian formulation exclusively. For more details see, for instance, Thurston (1964) and Wallace (1970, 1972).

1.3.6.3. Strain and stress tensors

The displacement vector from the reference position of a particle to its new position has as components

$$u_i = x_i - a_i. \quad (1.3.6.5)$$

The term strain refers to a change in the relative positions of the material points in a body. Let a final configuration be described in terms of the reference configuration by setting t equal to a constant in (1.3.6.1). Then t no longer appears as a variable and (1.3.6.1) can be written

$$x_i = x_i(a_1, a_2, a_3),$$

where the a_i are the independent variables. It follows that

$$dx_j = \frac{\partial x_j}{\partial a_i} da_i = \left(\frac{\partial u_j}{\partial a_i} + \delta_{ij} \right) da_i. \quad (1.3.6.6)$$

Let now the particle initially at (a_1, a_2, a_3) move to (x_1, x_2, x_3) . The square of the initial distance to a neighbouring particle whose initial coordinates were $a_j + da_j$ is

$$ds^2 = da_j da_j.$$

The square of the final distance to the same neighbouring particle is

$$ds^2 = dx_j dx_j.$$

In a material description, the strain components S_{ik} are defined by the following equations:

$$dx_j dx_j - da_j da_j = 2S_{ik} da_i da_k. \quad (1.3.6.7)$$

Substituting (1.3.6.6) into (1.3.6.7), it follows that

$$\left(\frac{\partial u_j}{\partial a_i} + \delta_{ji} \right) \left(\frac{\partial u_j}{\partial a_k} + \delta_{jk} \right) da_i da_k - da_j da_j = 2S_{ik} da_i da_k.$$

Hence

$$S_{ik} = \frac{1}{2} \left(\frac{\partial u_k}{\partial a_i} + \frac{\partial u_i}{\partial a_k} + \frac{\partial u_j}{\partial a_i} \frac{\partial u_j}{\partial a_k} \right).$$

If the products and squares of the displacement derivatives are neglected, the strain components reduce to the usual form of 'infinitesimal elasticity' [see equation (1.3.1.8)]:

$$S_{ik} = \frac{1}{2} \left(\frac{\partial u_i}{\partial a_k} + \frac{\partial u_k}{\partial a_i} \right).$$

It is often useful to introduce the Jacobian matrix associated with the transformation (\mathbf{a}, \mathbf{x}) . The components of this matrix are

$$J = \begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{pmatrix},$$

where

$$\alpha_{ik} = \frac{\partial x_i}{\partial a_k} = \frac{\partial u_j}{\partial a_k} + \delta_{jk}.$$

From the definition of matrix J , one has

$$d\mathbf{x} = J d\mathbf{a}$$

and

$$d\mathbf{x}^2 - d\mathbf{a}^2 = (d\mathbf{x})^T d\mathbf{x} - (d\mathbf{a})^T d\mathbf{a} = (d\mathbf{a})^T (J^T J - \delta) d\mathbf{a},$$

where $(d\mathbf{a})^T$, $(d\mathbf{x})^T$ and J^T are the transpose matrices of $d\mathbf{a}$, $d\mathbf{x}$ and J , respectively, and δ is the Kronecker matrix.

The Lagrangian strain matrix S may then be written symbolically:

$$S = \frac{1}{2} (J^T J - \delta). \quad (1.3.6.8)$$

When finite strains are concerned, we have to distinguish three states of the medium: the natural state, the initial state and the final or present state: The *natural* state is a state free of stress. The *initial* state is deduced from the natural state by a homogeneous strain. The *final* state is deduced from the initial state by an arbitrary strain.

1.3. ELASTIC PROPERTIES

Concerning the stress tensor, as pointed out by Thurston (1964), the stress-deformation relation is complicated in nonlinear elasticity because ‘the strain is often referred to a natural unstressed state, whereas the stress T_{ij} is defined per unit area of the deformed body’. For this reason, the differential of work done by the stress is not equal to the stress components times the differentials of the corresponding strain components. So, following Truesdell & Toupin (1960), we shall introduce a *thermodynamic tension tensor* t_{ij} defined as the first derivative of the energy with respect to strain. If the internal energy U per unit mass is considered, the *thermodynamic tension* refers to an isentropic process. Then

$$t_{ij}^{\sigma} = \rho_0 \left(\frac{\partial U}{\partial S_{ij}} \right)_{\sigma},$$

where σ is the entropy and ρ_0 the volumic mass in the initial state.

If the Helmholtz free energy F is considered, the thermodynamic tension refers to an isothermal process. Then

$$t_{ij}^{\Theta} = \rho_0 \left(\frac{\partial U}{\partial S_{ij}} \right)_{\Theta},$$

where Θ is the temperature. It will be shown in Section 1.3.7.2 that

$$T_{ij} = (1/J)\alpha_{ik}\alpha_{jl}t_{kl}.$$

1.3.6.4. Second-order and higher-order elastic stiffnesses

Following Brugger (1964), the strain-energy density, or strain energy per unit volume Φ , is assumed to be a polynomial in the strain:

$$\Phi = \Phi_0 + c_{ij}S_{ij} + \frac{1}{2!}c_{ijkl}S_{ij}S_{kl} + \frac{1}{3!}c_{ijklmn}S_{ij}S_{kl}S_{mn}, \quad (1.3.6.9)$$

where $\Phi = \rho_0 U(X, S_{ij})$, $\Phi_0 = \rho_0 U(X, 0)$, X denotes the configuration of the initial state and the S_{ij} 's are the Lagrangian finite strain-tensor components.

If the initial energy and the deformation of the body are both zero, the first two terms in (1.3.6.9) are zero. Note that c_{ij} is a stress and not an intrinsic characteristic of the material. In this expression, the elastic stiffnesses c_{ijkl} and c_{ijklmn} are the second- and third-order stiffnesses, respectively. Since the strain tensor is symmetric, pairs of subscripts can be interchanged [see equation (1.3.3.4)]:

$$\begin{aligned} c_{ijkl} &= c_{jikl} = c_{ijlk} = c_{jilk}, \\ c_{ijklmn} &= c_{jiklmn} = c_{ijlkmn} = c_{jilkmn} = c_{ijklmn} \\ &= c_{jiklmn} = c_{ijlkmn} = c_{jilkmn}. \end{aligned}$$

More accurately, the isentropic and the isothermal elastic stiffnesses are defined as the n th partial derivatives of the internal energy and the Helmholtz free energy, respectively. For example, the third-order isentropic and isothermal stiffnesses are, respectively,

$$\begin{aligned} c_{ijklmn}^{\sigma} &= \rho_0 \frac{\partial^3 U}{\partial S_{ij} \partial S_{kl} \partial S_{mn}}, \\ c_{ijklmn}^{\Theta} &= \rho_0 \frac{\partial^3 F}{\partial S_{ij} \partial S_{kl} \partial S_{mn}}, \end{aligned}$$

where the internal energy, U , is a function of X , S_{ij} and σ , and the Helmholtz free energy, F , is a function of X , S_{ij} and Θ .

From these definitions, it follows that the Brugger stiffness coefficients depend on the initial state. *When no additional information is given, the initial state is the natural state.*

Table 1.3.6.1. Number of independent third-order elastic stiffnesses for each Laue class

Laue class	Number of independent components
$\bar{1}, 1$	56
$2/m, 2, m$	32
$mmm, 222, 2mm$	20
$\bar{3}, 3$	20
$\bar{3}, 32, 3m$	14
$4/m, 4, \bar{4}$	16
$4/mmm, 422, \bar{4}2m, 42m$	12
$6/m, 6, \bar{6}$	12
$6/mmm, 622, \bar{6}2m, 62m$	10
$m\bar{3}, 23$	8
$m\bar{3}m, 432, \bar{4}32$	6
$\infty(A_{\infty}/M)C, \infty A_{\infty}$	3

The third-order stiffnesses form a sixth-rank tensor containing $3^6 = 729$ components, of which 56 are independent for a triclinic crystal and 3 for isotropic materials. The independent components of a sixth-rank tensor can be obtained for any point group using the accompanying software to this volume. They are listed in Table 1.3.6.1 for each Laue class. They can be reduced to three-index coefficients. Table 1.3.6.2 gives the values of the third-order stiffnesses of some materials.

The three independent constants for isotropic materials are often taken as c_{123} , c_{144} and c_{456} and denoted respectively by ν_1 , ν_2 , ν_3 , the ‘third-order Lamé constants’.

The ‘third-order Murnaghan constants’ (Murnaghan, 1951), denoted by l , m , n , are given in terms of the Brugger constants by the relations

$$l = \frac{1}{2}c_{112}; \quad m = c_{155}; \quad n = 4c_{456}.$$

Similarly, the fourth-order stiffnesses form an eighth-rank tensor containing $3^8 = 6561$ components, 126 of which are independent for a triclinic crystal and 11 for isotropic materials (the independent components of a sixth-rank tensor can be obtained for any point group using the accompanying software to this volume).

For a solid under finite strain conditions, the definition of the elastic compliance tensor has to be reconsidered. In linear elasticity, the second-order elastic compliances s_{ijkl} were defined through the relations (1.3.3.2):

$$S_{ij} = s_{ijkl}T_{kl} \quad \text{or} \quad s_{ijkl} = \frac{\partial S_{ij}}{\partial T_{kl}},$$

while, in nonlinear elasticity, one has

$$s_{ijkl} = \frac{\partial S_{ij}}{\partial t_{kl}},$$

where

$$t_{kl} = \rho_0 \frac{\partial U}{\partial S_{kl}}.$$

1.3.6.5. Expansion of elastic constants for small initial stress

In most experiments, the initial stress is small compared with the second-order elastic constants (for example, 1 GPa hydrostatic pressure compared with the usual value $c_{ijkl} = 100$ GPa). Consequently, the deformation between the initial (stressed) state and the natural (unstressed) state is small compared with 1. For this reason, it is convenient to expand the elastic constants in the initial state as a power series in the strain about the natural state. *To avoid confusion, we introduce new notations: \bar{X} now represents the coordinates in the natural or unstressed state; X represents the coordinates in the initial or homogeneously*

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Table 1.3.6.2. Third-order elastic stiffnesses of some materials in (GPa)⁻¹ (after Every & McCurdy, 1992)

(a) Trigonal.

Material	c ₁₁₁	c ₁₁₂	c ₁₁₃	c ₁₁₄	c ₁₂₃	c ₁₂₄	c ₁₃₃	c ₁₃₄	c ₁₄₄	c ₁₅₅	c ₂₂₂	c ₃₃₃	c ₃₄₄	c ₄₄₄
Al ₂ O ₃	-3870	-1090	-963	55	-289	-39	-922	-131	-302	-1160	-4520	-3340	-1090	-19
CaCO ₃	-579	-147	-193	218	-41	10	-239	82	-69	-139	-675	-498	-195	33

(b) Tetragonal.

Material	c ₁₁₁	c ₁₁₂	c ₁₁₃	c ₁₂₃	c ₁₃₃	c ₁₄₄	c ₁₅₅	c ₁₆₆	c ₃₃₃	c ₃₄₄	c ₃₆₆	c ₄₅₆
KH ₂ PO ₄	-538	-291	-259	-258	67	-8	-35	-30	-912	-27	-19	8
TeO ₂	-160	-600	-140	-110	180	-41	36	-640	-2110	-54	-260	-250

(c) Hexagonal.

Material	c ₁₁₁	c ₁₁₂	c ₁₁₃	c ₁₂₃	c ₁₃₃	c ₁₄₄	c ₁₅₅	c ₂₂₂	c ₃₃₃	c ₃₄₄
Cd	-2060	-114	-197	-110	-268	227	-332	-2020	-516	-171
CdS	-459	-207	-182	-235	-306	-27	9	-355	-327	-69
Co	-6710	-1454	-766	-429	-511	133	-1486	-5788	-6347	-210
Mg	-663	-178	30	-76	-86	-30	-58	-864	-726	-193
Zn	-1760	-440	-270	-210	-350	-10	250	-2410	-720	-440

(d) Cubic.

Material	c ₁₁₁	c ₁₁₂	c ₁₂₃	c ₁₄₄	c ₁₅₅	c ₄₅₆
LiF	-1920	-330	-40	100	-325	43
MgO	-4900	-95	-69	113	-659	147
KBr	-532	-49	69	22	-28	-35
KCl	-610	-31	9	19	-35	17
NaCl	-866	-37	38	25	-78	18
Diamond	-6260	-2260	112	-674	-2860	-823
GaAs	-620	-392	-62	8	-274	-43
Ge	-714	-388	-34	-9	-303	-48
Si	-795	-445	-75	15	-310	-86
ZnSe	-827	-136	-511	222	-265	-278
Al	-1224	-373	25	-64	-368	-27
Cu	-1271	-814	-50	-3	-780	-95
Au	-1730	-922	-233	-13	-648	-12
Fe	-2705	-626	-575	-836	-531	-721
Ni	-2104	-1345	59	-180	-757	-42

strained state; $u_i = x_i - X_i$ are the components of displacement. All letters with superscript bar refer to the natural state; for example, \bar{S}_{ij} denotes the Lagrangian strain in the natural state; $\bar{U} = \bar{U}(\bar{X}, \bar{S}_{ij})$.

Now, in order to relate the properties at X to those at \bar{X} , we need to specify the strain from \bar{X} to X . Let

$$a_{ij} = \frac{\partial X_i}{\partial \bar{X}_j} = \bar{\alpha}_{ij}.$$

Consequently,

$$\frac{\partial \bar{S}_{ij}}{\partial S_{mn}} = a_{mi} a_{nj}.$$

The second-order elastic constants at X can be expressed in terms of the second- and third-order elastic constants at \bar{X} :

$$c_{ijkl} = \rho_0 \frac{\partial^2 U}{\partial S_{ij} \partial S_{kl}} = \rho_0 \frac{\partial^2 \bar{U}}{\partial \bar{S}_{mn} \partial \bar{S}_{pq}} a_{im} a_{jn} a_{kp} a_{lq}$$

or

$$c_{ijkl} = \frac{\rho_0}{\rho_0} \left(\bar{c}_{mnpq} + \bar{c}_{mnpqrs} S_{rs} + \frac{1}{2!} \bar{c}_{mnpqrstuv} S_{rs} S_{tu} + \dots \right) a_{im} a_{jn} a_{kp} a_{lq}.$$

This expression holds for both isentropic and isothermal elastic constants.

1.3.6.6. Elastic strain-energy density

The elastic strain-energy density has appeared in the literature in various forms. Most of the authors use the Murnaghan constants as long as isotropic solids are concerned. However, most of the literature uses Brugger's thermodynamic definition when anisotropic media are under consideration (Brugger, 1964).

The elastic strain-energy density for an isotropic medium, including third-order terms but omitting terms independent of strain, may be expressed in terms of three strain invariants, since an isotropic material is invariant with respect to rotation:

$$\Phi = \frac{\lambda + 2\mu}{2} (I_1)^2 - 2\mu I_2 + \frac{l + 2m}{3} (I_1)^3 - 2m I_1 I_2 + n I_3,$$

where λ and μ are the second-order Lamé constants, l , m , n are the third-order Murnaghan constants, and I_1 , I_2 , I_3 are the three invariants of the Lagrangian strain matrix. These invariants may be written in terms of the strain components as

$$I_1 = S_{11} + S_{22} + S_{33}$$

$$I_2 = \begin{vmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{vmatrix} + \begin{vmatrix} S_{22} & S_{23} \\ S_{32} & S_{33} \end{vmatrix} + \begin{vmatrix} S_{33} & S_{31} \\ S_{13} & S_{11} \end{vmatrix}$$

$$I_3 = \begin{vmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{vmatrix}.$$

The elastic strain-energy density for an *anisotropic* medium (for example a medium belonging to the most symmetrical groups of cubic crystals) is (Green, 1973)

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$$\begin{aligned} \Phi = & \frac{1}{2}c_{11}[(S_{11})^2 + (S_{22})^2 + (S_{33})^2] + c_{12}[S_{11}S_{22} + S_{22}S_{33} + S_{33}S_{11}] \\ & + c_{44}[(S_{12})^2 + (S_{21})^2 + (S_{23})^2 + (S_{32})^2 + (S_{31})^2 + (S_{13})^2] \\ & + c_{111}[(S_{11})^3 + (S_{22})^3 + (S_{33})^3] \\ & + c_{112}[(S_{11})^2(S_{22} + S_{33}) + (S_{22})^2(S_{33} + S_{11}) \\ & + (S_{33})^2(S_{11} + S_{22})] \\ & + \frac{1}{2}c_{144}\{S_{11}[(S_{23})^2 + (S_{32})^2] + S_{22}[(S_{31})^2 + (S_{13})^2] \\ & + S_{33}[(S_{12})^2 + (S_{21})^2]\} \\ & + \frac{1}{2}c_{166}\{[(S_{12})^2 + (S_{21})^2](S_{11} + S_{22}) \\ & + [(S_{23})^2 + (S_{32})^2](S_{22} + S_{33}) \\ & + [(S_{13})^2 + (S_{31})^2](S_{11} + S_{33})\} \\ & + c_{123}S_{11}S_{22}S_{33} + c_{456}[S_{12}S_{23}S_{31} + S_{21}S_{32}S_{13}]. \end{aligned}$$

1.3.7. Nonlinear dynamic elasticity

1.3.7.1. Introduction

In recent years, the measurements of ultrasonic wave velocities as functions of stresses applied to the sample and the measurements of the amplitude of harmonics generated by the passage of an ultrasonic wave throughout the sample are in current use. These experiments and others, such as the interaction of two ultrasonic waves, are interpreted from the same theoretical basis, namely nonlinear dynamical elasticity.

A first step in the development of nonlinear dynamical elasticity is the derivation of the general equations of motion for elastic waves propagating in a solid under nonlinear elastic conditions. Then, these equations are restricted to elastic waves propagating either in an isotropic or in a cubic medium. The next step is the examination of two important cases:

(i) the generation of harmonics when *finite amplitude* ultrasonic waves travel throughout an *unstressed* medium;

(ii) the propagation of *small amplitude* ultrasonic waves when they travel throughout a *stressed* medium.

Finally, the concept of natural velocity is introduced and the experiments that can be used to determine the third- and higher-order elastic constants are described.

1.3.7.2. Equation of motion for elastic waves

For generality, these equations will be derived in the X configuration (initial state). It is convenient to obtain the equations of motion with the aid of Lagrange's equations. In the absence of body forces, these equations are

$$\frac{d}{dt} \frac{\partial L}{\partial x'_i} + \frac{\partial}{\partial X_i} \frac{\partial L}{\partial (\partial x_i / \partial X_j)} = 0 \quad (1.3.7.1)$$

or

$$\frac{d}{dt} \frac{\partial L}{\partial x'_i} + \frac{\partial}{\partial X_i} \frac{\partial L}{\partial \alpha_{ij}} = 0, \quad (1.3.7.2)$$

where L is the Lagrangian per unit initial volume and $\alpha_{ij} = \partial x_i / \partial X_j$ are the elements of the Jacobian matrix.

For adiabatic motion

$$L = \frac{1}{2} \rho_0 x_i'^2 - \rho_0 U, \quad (1.3.7.3)$$

where U is the internal energy per unit mass.

Combining (1.3.7.2) and (1.3.7.3), it follows that

$$\rho_0 x_i'' = \frac{\partial}{\partial X_j} \left(\rho_0 \frac{\partial U}{\partial S_{lm}} \frac{\partial S_{lm}}{\partial \alpha_{ij}} \right),$$

which can be written

$$\rho_0 x_i'' = \frac{\partial}{\partial X_j} \left(\alpha_{il} \alpha_{jm} \rho_0 \frac{\partial U}{\partial S_{lm}} \right)$$

since

$$\frac{\partial S_{lm}}{\partial \alpha_{ij}} = \frac{1}{2} (\alpha_{im} \delta_{jl} + \alpha_{il} \delta_{jm}).$$

Using now the equation of continuity or conservation of mass:

$$\frac{\rho_0}{\rho} = J = \det(a_{ij}),$$

and the identity of Euler, Piola and Jacobi:

$$\frac{\partial}{\partial x_j} \left(\frac{1}{J} \frac{\partial x_j}{\partial X_i} \right) = 0,$$

we get an expression of Newton's law of motion:

$$\rho x_i'' = \frac{dT_{ij}}{dX_j} \quad \text{or} \quad \rho u_i'' = \frac{dT_{ij}}{dX_j} \quad (1.3.7.4)$$

with

$$T_{ij} = \frac{\rho_0}{J} \alpha_{ik} \alpha_{jl} \frac{\partial U}{\partial S_{kl}} = \rho \alpha_{ik} \alpha_{jl} \frac{\partial U}{\partial S_{kl}}.$$

T_{ij} becomes

$$T_{ij} = \frac{1}{J} \alpha_{ik} \alpha_{jl} t_{kl}$$

since

$$t_{kl} = \rho_0 \frac{\partial U}{\partial S_{kl}}.$$

t_{kl} , the thermodynamic tensor conjugate to the variable S_{kl}/ρ_0 , is generally denoted as the 'second Piola-Kirchhoff stress tensor'.

Using Φ , the strain energy per unit volume, Newton's law (1.3.7.4) takes the form

$$\rho x_i'' = \frac{\partial}{\partial X_j} \left(\alpha_{jk} \frac{\partial \Phi}{\partial S_{ik}} \right) \quad \text{or} \quad \rho u_i'' = \frac{\partial}{\partial X_j} \left(\alpha_{jk} \frac{\partial \Phi}{\partial S_{ik}} \right)$$

and

$$T_{ij} = \alpha_{jk} \frac{\partial \Phi}{\partial S_{ik}}. \quad (1.3.7.5)$$

1.3.7.3. Wave propagation in a nonlinear elastic medium

As an example, let us consider the case of a plane finite amplitude wave propagating along the x_1 axis. The displacement components in this case become

$$u_1 = u_1(X_1, t); \quad u_2 = u_2(X_1, t); \quad u_3 = u_3(X_1, t).$$

Thus, the Jacobian matrix α_{ij} reduces to

$$J = \begin{pmatrix} \alpha_{11} & 0 & 0 \\ \alpha_{21} & 0 & 0 \\ \alpha_{31} & 0 & 0 \end{pmatrix}.$$

The Lagrangian strain matrix is [equation (1.3.6.8)]

$$S = \frac{1}{2} (J^T J - \delta).$$

The only nonvanishing strain components are, therefore,

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$$\begin{aligned}
 S_{11} &= \frac{1}{2}(\alpha_{11}^2 + \alpha_{21}^2 + \alpha_{31}^2) - 1 \\
 &= \frac{\partial u_1}{\partial X_1} + \frac{1}{2} \left[\left(\frac{\partial u_1}{\partial X_1} \right)^2 + \left(\frac{\partial u_2}{\partial X_1} \right)^2 + \left(\frac{\partial u_3}{\partial X_1} \right)^2 \right] \\
 S_{12} &= S_{21} = \frac{1}{2} \frac{\partial u_2}{\partial X_1} \\
 S_{13} &= S_{31} = \frac{1}{2} \frac{\partial u_3}{\partial X_1}
 \end{aligned}$$

and the strain invariants reduce to

$$I_1 = S_{11}; \quad I_2 = -(S_{12}S_{21} + S_{13}S_{31}); \quad I_3 = 0.$$

1.3.7.3.1. Isotropic media

In this case, the strain-energy density becomes

$$\begin{aligned}
 \Phi &= \frac{1}{2}(\lambda + 2\mu)(S_{11})^2 + 2\mu(S_{12}S_{21} + S_{13}S_{31}) + \frac{1}{3}(l + 2m)(S_{11})^3 \\
 &\quad + 2mS_{11}(S_{12}S_{21} + S_{13}S_{31}). \tag{1.3.7.6}
 \end{aligned}$$

Differentiating (1.3.7.6) with respect to the strains, we get

$$\begin{aligned}
 \frac{\partial \Phi}{\partial S_{11}} &= (\lambda + 2\mu)S_{11} + (l + 2m)(S_{11})^2 + 2m(S_{12}S_{21} + S_{13}S_{31}) \\
 \frac{\partial \Phi}{\partial S_{12}} &= 2\mu S_{21} + 2mS_{11}S_{21} \\
 \frac{\partial \Phi}{\partial S_{13}} &= 2\mu S_{31} + 2mS_{11}S_{31} \\
 \frac{\partial \Phi}{\partial S_{21}} &= 2\mu S_{12} + 2mS_{11}S_{12} \\
 \frac{\partial \Phi}{\partial S_{31}} &= 2\mu S_{13} + 2mS_{11}S_{13}.
 \end{aligned}$$

All the other $\partial \Phi / \partial S_{ij} = 0$.

From (1.3.7.5), we derive the stress components:

$$\begin{aligned}
 T_{11} &= \alpha_{1k} \frac{\partial \Phi}{\partial S_{1k}}; \quad T_{12} = \alpha_{2k} \frac{\partial \Phi}{\partial S_{1k}}; \quad T_{13} = \alpha_{3k} \frac{\partial \Phi}{\partial S_{1k}}; \\
 T_{21} &= \alpha_{1k} \frac{\partial \Phi}{\partial S_{2k}}; \quad T_{22} = \alpha_{2k} \frac{\partial \Phi}{\partial S_{2k}}; \quad T_{23} = \alpha_{3k} \frac{\partial \Phi}{\partial S_{2k}}; \\
 T_{31} &= \alpha_{1k} \frac{\partial \Phi}{\partial S_{3k}}; \quad T_{32} = \alpha_{2k} \frac{\partial \Phi}{\partial S_{3k}}; \quad T_{33} = \alpha_{3k} \frac{\partial \Phi}{\partial S_{3k}}.
 \end{aligned}$$

Note that this tensor is not symmetric.

For the particular problem discussed here, the three components of the equation of motion are

$$\begin{aligned}
 \rho u_1'' &= dT_{11}/dX_1, \\
 \rho u_2'' &= dT_{21}/dX_1, \\
 \rho u_3'' &= dT_{31}/dX_1.
 \end{aligned}$$

If we retain only terms up to the quadratic order in the displacement gradients, we obtain the following equations of motion:

$$\begin{aligned}
 \rho u_1'' &= (\lambda + 2\mu) \frac{\partial^2 u_1}{\partial X_1^2} + [3(\lambda + 2\mu) + 2(l + 2m)] \frac{\partial u_1}{\partial X_1} \frac{\partial^2 u_1}{\partial X_1^2} \\
 &\quad + (\lambda + 2\mu + m) \left[\frac{\partial u_2}{\partial X_1} \frac{\partial^2 u_2}{\partial X_1^2} + \frac{\partial u_3}{\partial X_1} \frac{\partial^2 u_3}{\partial X_1^2} \right] \\
 \rho u_2'' &= \mu \frac{\partial^2 u_2}{\partial X_1^2} + (\lambda + 2\mu + m) \left[\frac{\partial u_1}{\partial X_1} \frac{\partial^2 u_2}{\partial X_1^2} + \frac{\partial u_2}{\partial X_1} \frac{\partial^2 u_1}{\partial X_1^2} \right] \\
 \rho u_3'' &= \mu \frac{\partial^2 u_3}{\partial X_1^2} + (\lambda + 2\mu + m) \left[\frac{\partial u_1}{\partial X_1} \frac{\partial^2 u_3}{\partial X_1^2} + \frac{\partial u_3}{\partial X_1} \frac{\partial^2 u_1}{\partial X_1^2} \right]. \tag{1.3.7.7}
 \end{aligned}$$

1.3.7.3.2. Cubic media (most symmetrical groups)

In this case, the strain-energy density becomes

$$\begin{aligned}
 \Phi &= \frac{1}{2}c_{11}(S_{11})^2 + c_{44}[(S_{12})^2 + (S_{21})^2 + (S_{31})^2 + (S_{13})^2] \\
 &\quad + c_{111}(S_{11})^3 + \frac{1}{2}c_{166}S_{11}[(S_{12})^2 + (S_{21})^2 + (S_{31})^2 + (S_{13})^2]. \tag{1.3.7.8}
 \end{aligned}$$

Differentiating (1.3.7.8) with respect to the strain, one obtains

$$\begin{aligned}
 \frac{\partial \Phi}{\partial S_{11}} &= c_{11}S_{11} + 3c_{111}(S_{11})^2 + \frac{1}{2}c_{166}[(S_{12})^2 + (S_{21})^2 \\
 &\quad + (S_{31})^2 + (S_{13})^2] \\
 \frac{\partial \Phi}{\partial S_{21}} &= 2c_{44}S_{21} + c_{166}S_{11}S_{21} \\
 \frac{\partial \Phi}{\partial S_{31}} &= 2c_{44}S_{31} + c_{166}S_{11}S_{31}.
 \end{aligned}$$

All other $\partial \Phi / S_{ij} = 0$. From (1.3.7.5), we derive the stress components:

$$\begin{aligned}
 T_{11} &= \alpha_{1k} \frac{\partial \Phi}{\partial S_{1k}} \\
 T_{21} &= \alpha_{1k} \frac{\partial \Phi}{\partial S_{2k}} \\
 T_{31} &= \alpha_{1k} \frac{\partial \Phi}{\partial S_{3k}}.
 \end{aligned}$$

In this particular case, the three components of the equation of motion are

$$\begin{aligned}
 \rho u_1'' &= dT_{11}/dX_1 \\
 \rho u_2'' &= dT_{21}/dX_1 \\
 \rho u_3'' &= dT_{31}/dX_1.
 \end{aligned}$$

If we retain only terms up to the quadratic order in the displacement gradients, we obtain the following equations of motion:

$$\begin{aligned}
 \rho u_1'' &= c_{11} \frac{\partial^2 u_1}{\partial X_1^2} + [3c_{11} + c_{111}] \frac{\partial u_1}{\partial X_1} \frac{\partial^2 u_1}{\partial X_1^2} \\
 &\quad + (c_{11} + c_{166}) \left[\frac{\partial u_2}{\partial X_1} \frac{\partial^2 u_2}{\partial X_1^2} + \frac{\partial u_3}{\partial X_1} \frac{\partial^2 u_3}{\partial X_1^2} \right] \\
 \rho u_2'' &= c_{44} \frac{\partial^2 u_2}{\partial X_1^2} + (c_{11} + c_{166}) \left[\frac{\partial u_1}{\partial X_1} \frac{\partial^2 u_2}{\partial X_1^2} + \frac{\partial u_2}{\partial X_1} \frac{\partial^2 u_1}{\partial X_1^2} \right] \\
 \rho u_3'' &= c_{44} \frac{\partial^2 u_3}{\partial X_1^2} + (c_{11} + c_{166}) \left[\frac{\partial u_1}{\partial X_1} \frac{\partial^2 u_3}{\partial X_1^2} + \frac{\partial u_3}{\partial X_1} \frac{\partial^2 u_1}{\partial X_1^2} \right], \tag{1.3.7.9}
 \end{aligned}$$

which are identical to (1.3.7.7) if we put

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$$c_{11} = \lambda + 2\mu; \quad c_{44} = \mu; \quad c_{111} = 2(l + 2m); \quad c_{166} = m.$$

where u'_0 is the initial value for the particle velocity.

1.3.7.4. Harmonic generation

The coordinates in the medium free of stress are denoted either a or \bar{X} . The notation \bar{X} is used when we have to discriminate the natural configuration, \bar{X} , from the initial configuration X . Here, the process that we describe refers to the propagation of an elastic wave in a medium free of stress (natural state) and the coordinates will be denoted a_i .

Let us first examine the case of a pure longitudinal mode, *i.e.*

$$u_1 = u_1(a_1, t); \quad u_2 = u_3 = 0.$$

The equations of motion, (1.3.7.7) and (1.3.7.9), reduce to

$$\rho u_1'' = (\lambda + 2\mu) \frac{\partial^2 u_1}{\partial a_1^2} + [3(\lambda + 2\mu) + 2(l + 2m)] \frac{\partial u_1}{\partial a_1} \frac{\partial^2 u_1}{\partial a_1^2}$$

for an isotropic medium or

$$\rho u_1'' = c_{11} \frac{\partial^2 u_1}{\partial a_1^2} + [3c_{11} + c_{166}] \frac{\partial u_1}{\partial a_1} \frac{\partial^2 u_1}{\partial a_1^2}$$

for a cubic crystal (most symmetrical groups) when a pure longitudinal mode is propagated along [100].

For both cases, we have a one-dimensional problem; (1.3.7.7) and (1.3.7.9) can therefore be written

$$\rho u_1'' = K_2 \frac{\partial^2 u_1}{\partial a_1^2} + [3K_2 + K_3] \frac{\partial u_1}{\partial a_1} \frac{\partial^2 u_1}{\partial a_1^2}. \quad (1.3.7.10)$$

The same equation is also valid when a pure longitudinal mode is propagated along [110] and [111], with the following correspondence:

$$[100] \quad K_2 = c_{11}, \quad K_3 = c_{111}$$

$$[110] \quad K_2 = \frac{c_{11} + c_{12} + 2c_{44}}{2}, \quad K_3 = \frac{c_{111} + 3c_{112} + 12c_{166}}{4}$$

$$[111] \quad K_2 = \frac{c_{11} + 2c_{12} + 4c_{44}}{3},$$

$$K_3 = \frac{c_{111} + 6c_{112} + 12c_{144} + 24c_{166} + 2c_{123} + 16c_{456}}{9}.$$

Let us assume that $K_3 \ll K_2$; a perturbation solution to (1.3.7.10) is

$$u = u^0 + u^1,$$

where $u^1 \ll u^0$ with

$$u^0 = A \sin(ka - \omega t) \quad (1.3.7.11)$$

$$u^1 = Ba \sin 2(ka - \omega t) + Ca \cos 2(ka - \omega t). \quad (1.3.7.12)$$

If we substitute the trial solutions into (1.3.7.10), we find after one iteration the following approximate solution:

$$u = A \sin(ka - \omega t) - \frac{(kA)^2 (3K_2 + K_3)}{8\rho c^2} a \cos 2(ka - \omega t),$$

which involves second-harmonic generation.

If additional iterations are performed, higher harmonic terms will be obtained. A well known property of the first-order nonlinear equation (1.3.7.10) is that its solutions exhibit discontinuous behaviour at some point in space and time. It can be seen that such a discontinuity would appear at a distance from the origin given by (Breazeale, 1984)

$$L = -2 \frac{(K_2)^2}{3K_2 + K_3} \rho \omega u'_0,$$

where u'_0 is the initial value for the particle velocity.

1.3.7.5. Small-amplitude waves in a strained medium

We now consider the propagation of small-amplitude elastic waves in a homogeneously strained medium. As defined previously, \bar{X} or a are the coordinates in the natural or unstressed state. X are the coordinates in the initial or homogeneously strained state. $u_i = x_i - X_i$ are the components of displacement from the initial state due to the wave.

Starting from (1.3.7.4), we get

$$T_{ij} = \frac{\rho_0}{J} \alpha_{ik} \alpha_{jl} \frac{\partial U}{\partial S_{kl}}.$$

Its partial derivative is

$$\frac{\partial T_{ij}}{\partial x_j} = \frac{1}{J} \frac{\partial}{\partial X_k} \left[\rho_0 \alpha_{il} \frac{\partial U}{\partial S_{kl}} \right].$$

If we expand the state function about the initial configuration, it follows that

$$\begin{aligned} \rho_0 U(X_k, S_{ij}) &= \rho_0 U(X_k) + c_{ij} S_{ij} + \frac{1}{2} c_{ijkl} S_{ij} S_{kl} \\ &+ \frac{1}{6} c_{ijklmn} S_{ij} S_{kl} S_{mn} + \dots \end{aligned}$$

The linearized stress derivatives become

$$\frac{\partial T_{ij}}{\partial x_j} = [c_{jl} \delta_{ik} + c_{ijkl}] \frac{\partial^2 x_k}{\partial X_j \partial X_l}.$$

If we let $D_{ijkl} = [c_{jl} \delta_{ik} + c_{ijkl}]$, the equation of motion in the initial state is

$$\rho_0 u_i'' = D_{jkli} \frac{\partial^2 u_k}{\partial X_j \partial X_l}. \quad (1.3.7.13)$$

The coefficients D_{ijkl} do not present the symmetry of the coefficients c_{ijkl} except in the natural state where D_{ijkl} and c_{ijkl} are equal.

The simplest solutions of the equation of motion are plane waves. We now assume plane sinusoidal waves of the form

$$u_i = A_i \exp[i(\omega t - \mathbf{k} \cdot \mathbf{X})], \quad (1.3.7.14)$$

where \mathbf{k} is the wavevector.

Substitution of (1.3.7.14) into (1.3.7.13) results in

$$\rho_0 \omega^2 A_j = D_{ijkli} k_j k_l A_k$$

or

$$\rho_0 \omega^2 A_j = \Delta_{jk} A_k$$

with $\Delta_{jk} = D_{ijkli} k_j k_l$.

The quantities $\rho_0 \omega^2 A_j$ and A are, respectively, the *eigenvalues* and *eigenvectors of the matrix* Δ_{jk} . Since Δ_{jk} is a real symmetric matrix, the eigenvalues are real and the eigenvectors are orthogonal.

1.3.7.6. Experimental determination of third- and higher-order elastic constants

The main experimental procedures for determining the third- and higher-order elastic constants are based on the measurement of stress derivatives of ultrasonic velocities and on harmonic generation experiments. Hydrostatic pressure, which can be accurately measured, has been widely used; however, the measurement of ultrasonic velocities in a solid under hydrostatic pressure cannot lead to the whole set of third-order elastic constants, so uniaxial stress measurements or harmonic generation experiments are then necessary.

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Table 1.3.7.1. Relationships between ρW^2 , its pressure derivatives and the second- and third-order elastic constants

Propagation	Polarization	$(\bar{\rho}_0 W^2)_0$	$\partial(\bar{\rho}_0 W^2)_0/\partial p$
[100]	[100]	\bar{c}_{11}	$-1 - (2\bar{c}_{11} + \Gamma_{1111})/3\bar{\kappa}$
[100]	[010]	\bar{c}_{44}	$-1 - (2\bar{c}_{44} + \Gamma_{2323})/3\bar{\kappa}$
[110]	[110]	$(\bar{c}_{11} + \bar{c}_{12} + 2\bar{c}_{44})/2$	$-1 - (\bar{c}_{11} + \bar{c}_{12} + 2\bar{c}_{44} + 0.5[\Gamma_{1111} + \Gamma_{1122} + \Gamma_{2323}])/3\bar{\kappa}$
[110]	[110]	$(\bar{c}_{11} - \bar{c}_{12} + \bar{c}_{44})/3$	$-1 - (\bar{c}_{11} - \bar{c}_{12} + 0.5[\Gamma_{1111} - \Gamma_{1122}])/3\bar{\kappa}$
[110]	[001]	\bar{c}_{44}	$-1 - (2\bar{c}_{44} + \Gamma_{2323})/3\bar{\kappa}$
[111]	[111]	$(\bar{c}_{11} + 2\bar{c}_{12} + 4\bar{c}_{44})/3$	$-1 - (2\bar{c}_{11} + 4\bar{c}_{12} + 8\bar{c}_{44} + [\Gamma_{1111} + 2\Gamma_{1122} + 4\Gamma_{2323}])/9\bar{\kappa}$
[111]	[110]	$(\bar{c}_{11} - \bar{c}_{12} + \bar{c}_{44})/3$	$-1 - (2\bar{c}_{11} - 2\bar{c}_{12} + 2\bar{c}_{44} + [\Gamma_{1111} - \Gamma_{1122} + \Gamma_{2323}])/9\bar{\kappa}$

In order to interpret wave-propagation measurements in stressed crystals, Thurston (1964) and Brugger (1964) introduced the concept of natural velocity with the following comments:

‘According to equation of motion, the wave front is a material plane which has unit normal \mathbf{k} in the natural state; a wave front moves from the plane $\mathbf{k} \cdot \mathbf{a} = \mathbf{0}$ to the plane $\mathbf{k} \cdot \mathbf{a} = \mathbf{L}_0$ in the time L_0/W . Thus W , the natural velocity, is the wave speed referred to natural dimensions for propagation normal to a plane of natural normal \mathbf{k} .

In a typical ultrasonic experiment, plane waves are reflected between opposite parallel faces of a specimen, the wave fronts being parallel to these faces. One ordinarily measures a repetition frequency F , which is the inverse of the time required for a round trip between the opposite faces.’

Hence

$$W = 2L_0F.$$

In most experiments, the third-order elastic constants and higher-order elastic constants are deduced from the stress derivatives of $\bar{\rho}_0 W^2$. For instance, Table 1.3.7.1 gives the expressions for $(\bar{\rho}_0 W^2)_0$ and $\partial(\bar{\rho}_0 W^2)_0/\partial p$ for a cubic crystal. These quantities refer to the natural state free of stress. In this table, p denotes the hydrostatic pressure and the Γ_{ijkl} 's are the following linear combinations of third-order elastic constants:

$$\begin{aligned}\Gamma_{1111} &= \bar{c}_{111} + 2\bar{c}_{111} \\ \Gamma_{1122} &= 2\bar{c}_{112} + \bar{c}_{123} \\ \Gamma_{2323} &= \bar{c}_{144} + 2\bar{c}_{166}.\end{aligned}$$

1.3.8. Glossary

\mathbf{e}_i	covariant basis vector
A^T	transpose of matrix A
u_i	components of the displacement vector
S_{ij}	components of the strain tensor
S_α	components of the strain Voigt matrix
T_{ij}	components of the stress tensor
T_α	components of the stress Voigt matrix
p	pressure
\mathbf{v}	normal stress
$\boldsymbol{\tau}$	shear stress
s_{ijkl}	second-order elastic compliances
$s_{\alpha\beta}$	reduced second-order elastic compliances
$(s_{ijkl})^\sigma$	adiabatic second-order elastic compliances
s_{ijklmn}	third-order elastic compliances
c_{ijkl}	second-order elastic stiffnesses
$(c_{ijkl})^\sigma$	adiabatic second-order elastic stiffnesses
$c_{\alpha\beta}$	reduced second-order elastic stiffnesses
c_{ijklmn}	third-order elastic stiffnesses
ν	Poisson's ratio
E	Young's modulus
κ	bulk modulus (volume compressibility)

λ, μ	Lamé constants
Θ	temperature
c^s	specific heat at constant strain
ρ	volumic mass
Θ_D	Debye temperature
k_B	Boltzmann constant
U	internal energy
F	free energy

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