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Lecture-21

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2.11 Dynamics of the Nuclei at Large Wavelengths

This section is concerned with the vibrational modes whose wavelength is much larger than the diameter of the elementary cell of the direct lattice. As shown in Sect. 2.9, in the acoustic branches the group velocity coincides with the phase velocity when q is small; this means that a wave packet made of the superposition of low-q waves propagates within the crystal without being distorted. Also, remembering that $q = 2\pi/\lambda$, a small value of q corresponds to a long wavelength; in such a condition, the atomic nature of the crystal has little importance for the dynamics of the displacements: the crystal, in fact, may be considered as a continuous medium. Such a situation is typical of the propagation of the sound waves in a solid: the motion of the nuclei in the case of acoustic branches is such, that the nuclei of each elementary cell move as a single block.[15] This makes it possible to simplify the description of the dynamics of the nuclei: the starting point is the general expression (2.73) of the force, whence the dynamics of each component u of the αth nucleus of the mth cell is given by

$$\mu_\alpha \ddot{h}_{m\alpha u} = -\sum_{n=1}^{N_c}\sum_{\beta=1}^{N_b}\sum_{w=1}^{3} c_{m\alpha u}^{n\beta w}\, h_{n\beta w}\,. \tag{2.88}$$

For an acoustic mode, the nuclei of each cell move as a single block, whence one may let

$$\psi_{mu} = h_{m1u} = h_{m2u} = \ldots\,, \qquad \psi_{nw} = h_{n1w} = h_{n2w} = \ldots\,. \tag{2.89}$$

Adding up over α both sides of (2.89) yields

$$\sum_{\alpha=1}^{N_b} \mu_\alpha \ddot{h}_{m\alpha u} = M\ddot{\psi}_{mu} = -\sum_{n=1}^{N_c}\sum_{\alpha,\beta=1}^{N_b}\sum_{w=1}^{3} c_{m\alpha u}^{n\beta w}\,\psi_{nw} = -\sum_{n=1}^{N_c}\sum_{w=1}^{3} Q_{mu}^{nw}\,\psi_{nw}\,, \tag{2.90}$$

with

$$M = \sum_{\alpha=1}^{N_b} \mu_\alpha\,, \qquad Q_{mu}^{nw} = \sum_{\alpha,\beta=1}^{N_b} c_{m\alpha u}^{n\beta w}\,, \tag{2.91}$$

M being the total mass of each cell: in other terms, the lattice is treated as if it were monatomic. Since the elastic matrix $\mathbf{C}$, whose entries are $c_{m\alpha u}^{n\beta w}$, is positive definite (Sect. 2.2), then the matrix of entries Q_{mu}^{nw} defined in (2.91) is positive definite as well (Prob. 2.6). Note that due to the coordinate-inversion invariance it is

$$Q_{nu}^{mw} = Q_{mu}^{nw}\,, \qquad Q_{nu}^{0w} = Q_{0u}^{nw}\,, \qquad Q_u^w(-\mathbf{l}_n) = Q_u^w(\mathbf{l}_n)\,. \tag{2.92}$$

In the above it is $\psi_{mu} = \psi_u(\mathbf{l}_m)$, $\psi_{nw} = \psi_w(\mathbf{l}_n)$. When the long-wavelength modes are considered, the crystal may be treated as a continuous medium; for this reason,

[15] In contrast, in the case of optical branches the nuclei belonging to the same elementary cell have also a motion relative to each other.

Coordinate invariance

Translational Invariance

Invariance upon Reflection

the translational vectors $\mathbf{l}_m$, $\mathbf{l}_n$ are replaced when necessary with the continuous position variable $\mathbf{r}$. In the same order of approximation, one may assume that the displacement at the mth or nth cell varies little with respect to that in the origin: this allows one to expand $\psi_w(\mathbf{l}_n)$ around $\mathbf{l}_0 = 0$ at the right hand side of (2.90); truncating the expansion to second order yields

$$\psi_w(\mathbf{l}_n) \simeq \psi_w(0) + \sum_{i=1}^{3} \left(\frac{\partial \psi_w}{\partial x_i}\right)_0 l_{ni} + \frac{1}{2} \sum_{i,j=1}^{3} \left(\frac{\partial^2 \psi_w}{\partial x_i \, \partial x_j}\right)_0 l_{ni} \, l_{nj} \,, \tag{2.93}$$

Linear Monoatomicchain

so that (2.90) becomes

$$M \, \ddot{\psi}_u(\mathbf{l}_m) = - \sum_{n=1}^{N_c} \sum_{w=1}^{3} Q_{mu}^{nw} \left[\psi_w(0) + \overbrace{\sum_{i=1}^{3} (\ldots) \, l_{ni}}^{=0} + \overbrace{\frac{1}{2} \sum_{i,j=1}^{3} (\ldots) \, l_{ni} \, l_{nj}}^{=0} \right] , \tag{2.94}$$

where the dots stand for the coefficients of (2.93). The right hand side of (2.94) simplifies greatly thanks to some of the invariance properties demonstrated in Sect. 2.10. The first term at the right hand side vanishes due to translational invariance (2.77):

$$\boxed{\sum_{n=1}^{N_c} \sum_{w=1}^{3} Q_{mu}^{nw} \, \psi_w(0) = \sum_{\alpha=1}^{N_b} \sum_{w=1}^{3} \left(\sum_{n=1}^{N_c} \sum_{\beta=1}^{N_b} c_{m\alpha u}^{n\beta w} \right) \psi_w(0) = 0 .} \tag{2.95}$$

As for the second term at the right hand side of (2.94) one finds

$$\sum_{n=1}^{N_c} \sum_{w=1}^{3} Q_{mu}^{nw} \sum_{i=1}^{3} \left(\frac{\partial \psi_w}{\partial x_i}\right)_0 l_{ni} = \sum_{w,i=1}^{3} \left(\frac{\partial \psi_w}{\partial x_i}\right)_0 \sum_{n=1}^{N_c} Q_{mu}^{nw} \, l_{ni} \,, \tag{2.96}$$

where one may replace index m with 0 by choosing the mth node as the coordinate origin. In addition, due to the crystal periodicity one may also make the coordinate origin to coincide with the center of the crystal. As a consequence, the sum over n in (2.96) splits into terms of the form

$$Q_u^w(\mathbf{l}_n) \, l_{ni} + Q_u^w(-\mathbf{l}_n) \, (-l_{ni}) = 0 \,, \tag{2.97}$$

whose vanishing is due to the coordinate-inversion invariance (2.92). In conclusion, the dynamical relation (2.94) reduces to

$$\boxed{M \, \ddot{\psi}_u(\mathbf{l}_m) = - \sum_{n=1}^{N_c} \sum_{w=1}^{3} Q_{0u}^{nw} \, \frac{1}{2} \sum_{i,j=1}^{3} \left(\frac{\partial^2 \psi_w}{\partial x_i \, \partial x_j}\right)_0 l_{ni} \, l_{nj} .} \tag{2.98}$$

2.12 Elastic Tensor

The simplified form (2.98) of the dynamical relation, applicable to the vibrational modes of large wavelength, is further simplified as shown below. First, the dependence on $\mathbf{l}_m$ is replaced with the dependence on the continuous position variable $\mathbf{r}$; second, suffix 0 of the second derivative is dropped, on account of the fact that the spatial derivatives of the displacements vary little within the crystal. Next, let Ω indicate the crystal volume; the density of the material is given by

$$\rho = \frac{N_c M}{\Omega} = \frac{M}{\Omega / N_c} = \frac{M}{\tau_l}, \tag{2.99}$$

with τ_l the volume of the lattice cell. Such a density is that of the $\psi_u = 0$ case; in fact, it is assumed that ρ is not affected by the displacements because the latter are small. Dividing both sides of (2.98) by τ_l, and defining the rank-4 *elastic tensor*

$$\boxed{\Phi^{ij}_{uw} = -\frac{1}{2\,\tau_l} \sum_{n=1}^{N_c} Q^{nw}_{0u}\, l_{ni}\, l_{nj}}\,, \tag{2.100}$$

one finds

$$\boxed{\rho\, \ddot{\psi}_u = \sum_{w=1}^{3} \sum_{i,j=1}^{3} \Phi^{ij}_{uw} \frac{\partial^2 \psi_w}{\partial x_i\, \partial x_j}}\,. \tag{2.101}$$

The elastic tensor has $3^4 = 81$ components, which can be arranged into a 9×9 matrix as shown in Fig. 2.6. The rows of the matrix correspond to the 9 combinations of the u, w indices, while the columns correspond to the 9 combinations of the i, j indices. By construction, Φ^{ij}_{uw} is invariant upon exchange of i and j: this means that

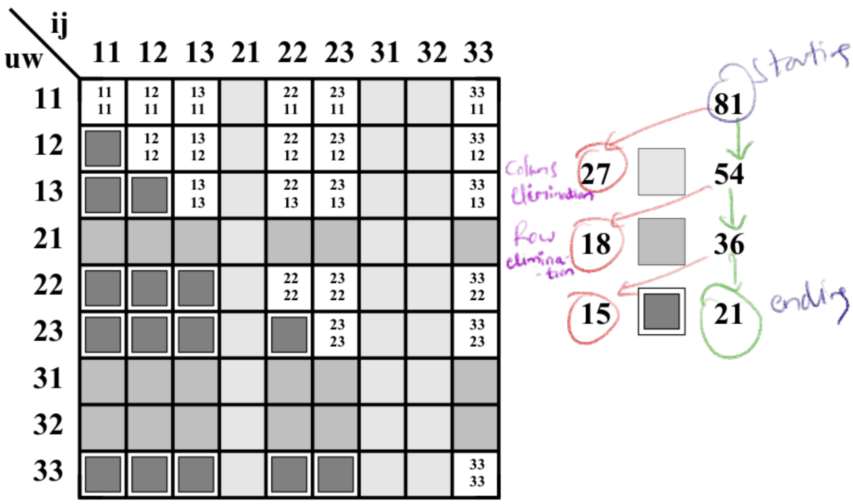

Fig. 2.6 Schematic view of the 9×9 matrix representing the elastic tensor. The different intensities of gray aim at describing the reasoning that, by successive reductions, brings the number of independent entries to 21 (the explanation is given in the text). In the right part of the figure, numbers 27, 18, and 15 indicate the number of entries marked in light, medium, and dark gray, respectively; numbers 81, 54, 36, 21 indicate the number of independent entries left after each reduction

three columns, say, those of indices 21, 31, 32, are respectively identical to those of indices 12, 13, 23; such columns are those marked in light gray in Fig. 2.6. The number of indipendent entries of the matrix thus reduces to $81 - 3 \times 9 = 54$, and the number of independent entries of each row reduces to 6.

Then, remembering that Q^{nw}_{mu} has the same type of symmetry as $c^{n\beta w}_{m\alpha u}$, one finds that the elastic tensor is invariant also when u and w are exchanged. In fact, from $c^{m\alpha u}_{n\beta w} = c^{n\beta w}_{m\alpha u}$ it follows $Q^{0u}_{nw} = Q^{nw}_{0u}$ whence $\Phi^{ij}_{wu} = \Phi^{ij}_{uw}$. This means that three rows, say, those of indices 21, 31, 32, are respectively identical to those of indices 12, 13, 23; such columns are those marked in medium gray in Fig. 2.6. The number of indipendent entries thus reduces to $54 - 3 \times 6 = 36$, and can be arranged into a 6×6 matrix.

If the 6×6 matrix thus found is symmetric, the number of independent entries is further reduced; specifically, the number of non-diagonal entries is $36 - 6 = 30$ but, if the matrix is symmetric, only $30/2 = 15$ of the latter are independent. The 15 non-independent entries identified at this stage are those marked in dark gray in Fig. 2.6. Adding back the diagonal elements one finally finds that the number of independent entries of a symmetric 6×6 matrix is $15 + 6 = 21$. When this type of symmetry occurs, the elastic tensor is invariant under the exchange of the two pairs of indices ij and uw.

It may be shown that the symmetry of the 6×6 matrix always holds, regardless of the type of the crystal; in fact all steps, involved so far in the reduction of the independent entries from 81 to 21, have exploited the periodicity properties of the lattice and the definition of the elastic tensor, without ever taking any other property of the crystal into account. To proceed, one may seek for additional invariance properties; an important one, not exploited yet, is that the interatomic forces are of the central type: due to this, it can be shown that all indices u, w, i, j are in fact interchangeable (the demonstration is in Prob. 2.7). It follows that, out of the 21 independent entries considered so far, those whose sets of four indices differ by a permutation are in fact equal. Such entries are

$$\Phi^{11}_{22} = \Phi^{12}_{12}\,, \quad \Phi^{11}_{23} = \Phi^{12}_{13}\,, \quad \Phi^{11}_{33} = \Phi^{13}_{13}\,, \tag{2.102}$$

$$\Phi^{12}_{23} = \Phi^{13}_{22}\,, \quad \Phi^{12}_{33} = \Phi^{13}_{23}\,, \quad \Phi^{22}_{33} = \Phi^{23}_{23}\,. \tag{2.103}$$

Due to (2.102, 2.103), the number of independent entries decreases by 6. In conclusion, when the interatomic forces are of the central type the number of independent entries of the elastic tensor is $21 - 6 = 15$. Such a number may be decreased even further if particular symmetries exist in the crystal under investigation (Sect. 2.17).

Forces of the Central Type — IX

The minimum number of independent entries is 3, that occurs in the cubic crystals. In such a case the only non-vanishing entries are

$$\Phi^{11}_{11} = \Phi^{12}_{12} = \Phi^{13}_{13} = \Phi_a\,, \quad \Phi^{22}_{22} = \Phi^{23}_{23} = \Phi^{33}_{33} = \Phi_b\,,$$

$$\Phi^{11}_{12} = \Phi^{11}_{13} = \Phi^{12}_{11} = \Phi^{12}_{13} = \Phi^{13}_{11} = \Phi^{13}_{12} = \Phi_c\,,$$

and the 6×6 form of the elastic tensor becomes

$$\begin{bmatrix} \Phi_a & \Phi_c & \Phi_c & 0 & 0 & 0 \\ \Phi_c & \Phi_a & \Phi_c & 0 & 0 & 0 \\ \Phi_c & \Phi_c & \Phi_a & 0 & 0 & 0 \\ 0 & 0 & 0 & \Phi_b & 0 & 0 \\ 0 & 0 & 0 & 0 & \Phi_b & 0 \\ 0 & 0 & 0 & 0 & 0 & \Phi_b \end{bmatrix}$$

2.13 Strain and Stress Tensors

Consider the case discussed at the end of Sect. 2.12, where all indices of Φ^{ij}_{uw} are interchangeable; due to this, there are permutations of indices that leave (2.101) unchanged: in particular,

density multiplied by Acceleration along one of the 3 directions

$$\rho\,\ddot{\psi}_u = \sum_{w,i,j=1}^{3} \Phi^{ij}_{uw} \frac{\partial^2 \psi_w}{\partial x_i \partial x_j} = \sum_{w,i,j=1}^{3} \Phi^{wj}_{ui} \frac{\partial^2 \psi_w}{\partial x_i \partial x_j} = \sum_{w,i,j=1}^{3} \Phi^{ij}_{uw} \frac{\partial^2 \psi_i}{\partial x_w \partial x_j}\,. \tag{2.104}$$

The same term $\rho\,\ddot{\psi}_u$ is equally well expressed after exchanging indices i and j in the sums at the right hand side; adding (2.104) to the new expression thus found, and dividing by 2 yield, after splitting the derivatives and rearranging the indices,

$$\rho\,\ddot{\psi}_u = \sum_{w,i,j=1}^{3} \frac{\partial}{\partial x_w}\left(\frac{1}{2}\Phi^{ij}_{uw}\frac{\partial \psi_i}{\partial x_j} + \frac{1}{2}\Phi^{ji}_{uw}\frac{\partial \psi_j}{\partial x_i}\right) = \tag{2.105}$$

$$= \sum_{w=1}^{3} \frac{\partial}{\partial x_w} \sum_{i,j=1}^{3} \Phi^{ij}_{uw}\,\frac{1}{2}\left(\frac{\partial \psi_i}{\partial x_j} + \frac{\partial \psi_j}{\partial x_i}\right).$$

The above is recast in a more compact form as

Strain Tensor

$$\rho\,\ddot{\psi}_u = \sum_{w=1}^{3} \frac{\partial}{\partial x_w} \sum_{i,j=1}^{3} \Phi^{ij}_{uw}\,\varepsilon_{ij}\,, \qquad \boxed{\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial \psi_i}{\partial x_j} + \frac{\partial \psi_j}{\partial x_i}\right)}\,, \tag{2.106}$$

with ε_{ij} the *strain tensor*. By construction, the strain tensor is symmetric; also, its components are dimensionless: from the latter property it follows that the ratio between the components of the elastic tensor Φ^{ij}_{uw} and a length is homogeneous with $\rho\,\ddot{\psi}_u$, whose dimensions are those of a force per unit volume. In conclusion, the dimensions of the elastic tensor are those of a force per unit area, that is, a stress. Defining the *stress tensor* as

Relation b/w Stress & Strain Tensor

$$\boxed{\sigma_{uw} = \sum_{i,j=1}^{3} \Phi^{ij}_{uw}\,\varepsilon_{ij}}\,, \tag{2.107}$$

divergence of stress Tensor

gives (2.106) the final form

$$\boxed{\rho\,\ddot{\psi}_u = \sum_{w=1}^{3} \frac{\partial \sigma_{uw}}{\partial x_w}}\,. \tag{2.108}$$

Since the strain tensor is dimensionless, the units of σ_{uw} are the same as those of Φ^{ij}_{uw}; also, σ_{uw} is a symmetric tensor because Φ^{ij}_{uw} is invariant when u and w are exchanged. In conclusion, (2.108) provides the dynamical description of the acoustic modes in the long-wavelength limit, in the hypothesis that the interatomic forces are of the central type; a comparison with (2.126) shows that (2.108) coincides with the elasticity law of a continuous medium.

Hooke's law of Elasticity for an anisotropic medium $\Rightarrow$ Elongation $\propto$ Applied force

Due to symmetry, the 3×3 strain tensor ε_{ij} and, similarly, the 3×3 stress tensor σ_{uw} have 6 independent entries; such entries are generally recast in the form of a 6×1 vector according to the following scheme:

$$\begin{bmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{bmatrix} = \begin{bmatrix} \mathbf{11} & \mathbf{12} & 31 \\ 12 & \mathbf{22} & \mathbf{23} \\ \mathbf{31} & 23 & \mathbf{33} \end{bmatrix} \Rightarrow \begin{bmatrix} \mathbf{11} \\ \mathbf{22} \\ \mathbf{33} \\ \mathbf{23} \\ \mathbf{31} \\ \mathbf{12} \end{bmatrix} \Rightarrow \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{bmatrix}, \tag{2.109}$$

where indices in bolface indicate the independent entries. The same method for compacting the indices is applied to the elastic tensor Φ_{uw}^{ij}: for this, one refers again to Fig. 2.6, specifically to the entries that, after the reduction from 81 to 21, have been left white; noting that each of these entries is marked with the corresponding pairs of indices u, w and i, j, one replaces each pair with a single index following the scheme indicated in (2.109). At the end of the replacement, the indices of the 21 entries are such that, exploiting the $u, w \leftrightarrow i, j$ invariance, one obtains a 6×6, symmetric matrix $\mathbf{B}$ of elements b_{pq}, with p replacing u, w and q replacing i, j; in conclusion, (2.107) transforms into (2.110), shown below, where, like in (2.109), the independent entries are in boldface. Note that at this stage the reduction in the number of independent entries due to the properties of the central forces has not taken place yet; using (2.102, 2.103), a further reduction from 21 to 15 of the independent entries is achieved. Matrix $\mathbf{B}$ of (2.110) is called *stiffness matrix*, and its units are the same as those of Φ_{uw}^{ij}, namely, a force per unit area. In the following it is assumed that $\mathbf{B}$ is nonsingular;[16] therefore, its inverse $\mathbf{H} = \mathbf{B}^{-1}$ exists, and is called *compliance matrix*. Since $\mathbf{B}$ is symmetric, $\mathbf{H}$ is symmetric as well (Prob. 2.8).

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} \mathbf{b_{11}} & \mathbf{b_{12}} & \mathbf{b_{13}} & \mathbf{b_{14}} & \mathbf{b_{15}} & \mathbf{b_{16}} \\ b_{21} & \mathbf{b_{22}} & \mathbf{b_{23}} & \mathbf{b_{24}} & b_{25} & b_{26} \\ b_{31} & b_{32} & \mathbf{b_{33}} & b_{34} & b_{35} & b_{36} \\ b_{41} & b_{42} & \mathbf{b_{43}} & \mathbf{b_{44}} & b_{45} & b_{46} \\ b_{51} & \mathbf{b_{52}} & \mathbf{b_{53}} & \mathbf{b_{54}} & \mathbf{b_{55}} & b_{56} \\ b_{61} & \mathbf{b_{62}} & \mathbf{b_{63}} & \mathbf{b_{64}} & \mathbf{b_{65}} & \mathbf{b_{66}} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}. \tag{2.110}$$

Equation (2.107) expresses the stress components (that are forces per unit area) as linear combinations with constant coefficients of the strain components. Linearity is not a general properties of materials; here it is a consequence of a number of approximations, namely, that the components of the elastic tensor are calculated assuming that the spatial derivatives of the displacements vary little within the crystal, and that the displacements themselves are small (Sect. 2.12). It is interesting to note

[16] In theory it is possible to construct cases in which a null strain vector corresponds to a non-null stress vector, or viceversa. This, however, does not happen in real materials.

that (2.107) is the generalization of *Hooke's law* to an anisotropic medium (see also the comments at p. 108).[17]

2.14 Connection with the Macroscopic Theory

The analysis carried out in Sects. 2.1 through 2.13 has dealt with a system of N interacting particles, for which it was assumed that the displacements with respect to the equilibrium point were small; this situation is typical of solid materials. Then, assuming that the external forces were absent, the analysis concentrated on describing the vibrational modes of the particles; the calculation was greatly simplified by the hypothesis that the material was a crystal: in fact, exploiting the periodicity of the structure limits the analysis to a single spatial period.

The dynamics of the acoustic modes at large wavelengths was given special consideration in Sect. 2.11, to eventually lead to the definition of the strain and stress tensors, and to the relation (2.107) between the two; this relation is linear thanks to a number of approximations listed in Sect. 2.13. Finally, the dynamical law (2.108) describing the displacements of the acoustic modes in the long-wavelength limit was worked out, in the hypothesis that the interatomic forces are of the central type.

In summary, the approach of Sects. 2.1–2.13 follows the "bottom-up" scheme, starting from the interactions among atoms and deriving from them some macroscopic properties. On the other hand, some of the relations deduced in the preceding sections can also be worked out directly from macroscopic considerations: this part of the analysis is the object of the remaining part of the chapter. As shown below, the hypothesis of the absence of external forces is not made any more; given a block of material, different external forces may be present simultaneously: some are applied to the body of the material (e.g., gravity), others are applied to its external surface; among the latter are the pressure, due for instance to immersion of the material in a fluid; in other instances, the surface forces are those exerted by other portions of the structure to which the block belongs, and may produce compression, bending, and/or twisting of the block itself. In some cases, the surface forces are produced by the attempt of the block to expand or shrink due to a change in temperature.

The starting point for the discussion is a prismatic block of material of sides a_1, a_2, a_3 (Fig. 2.7). For the typical applications considered here, the block sketched in the figure represents a solid-state device or a part of it; therefore, the linear dimensions of the physical system under investigation are still large enough to treat the system as a continuous body.[18] It is also important to point out that, as the size of the system

[17] R. Hooke (1635–1703) first mentioned the law in 1676 as an anagram, *ceiiinosssttuv*; he explained it in 1678 as *ut (ex)tensio sic vis*, a Latin sentence meaning "as the extension, so the force" [27].

[18] By way of example, a state-of-the-art micro-electro-mechanical (MEM) structure may have a length of 50 nm, whereas the lattice constant of a semiconductor like silicon is of the order of 0.5 nm.

Q) what happens when This Block of material is subjected to External force ?

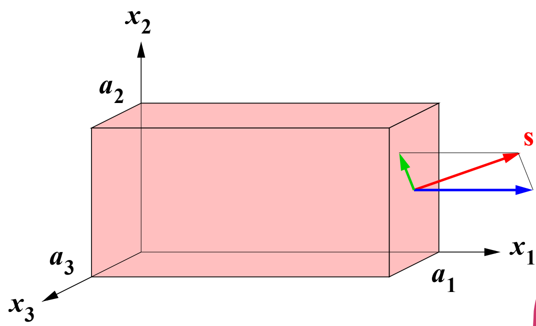

Fig. 2.7 A prismatic block of material of sides a_1, a_2, a_3. The red arrow shows the stress $\mathbf{s} = \lim_{A\to 0} \mathbf{F}/A$, with A the area of the face (here $A = a_2\, a_3$). The blue arrow is the projection of the stress along the direction normal to the face, while the green arrow is the projection over the face. The same structure of vectors (not drawn in the figure) applies to all remaining faces

Jump to Deformation

becomes smaller, the effect of the surface forces becomes more and more relevant with respect to that of the body forces: taking by way of example a cube of material of side L, the surface/volume ratio is 6 m^{-1} when $L = 1$ m, while it becomes 600 m^{-1} when $L = 1$ cm, and 6×10^6 m^{-1} when $L = 1$ μm.

Assume that the prismatic block shown in Fig. 2.7 is placed in the interior of a larger body, and that it is subjected to external actions; apart from gravity, which is not considered for the moment, such actions derive from forces applied to the external surface of the body to which the block belongs: as a consequence, the external forces are transferred from the surface of the body through the internal parts, and eventually reach the faces of the block. Given that, one may think of isolating the block from the rest of the body: if this is done, after removing the rest of the body one must apply to each face of the block the same action that was originally exerted by the body.

In the most general case, such an action is made, for each face, of the combination of a force $\mathbf{F}$ and a torque $\mathbf{M}$; both depend on the area A of the face and on its orientation. Since the block is assumed to be small, it is sensible to consider the limits

$$\mathbf{s} = \lim_{A\to 0} \frac{\mathbf{F}}{A}\,, \qquad\qquad \mathbf{m} = \lim_{A\to 0} \frac{\mathbf{M}}{A}\,. \tag{2.111}$$

It is found that the latter limit vanishes, whereas the former is typically finite: it provides a force per unit area which, as already mentioned in Sect. 2.13, is called *stress* (or *tension*).[19] The stress acting on the right face of the block is shown as the red arrow in Fig. 2.7 (for the sake of simplicity, the stresses acting on the other faces are not drawn); such a stress is not necessarily normal to the face: its projection along the direction normal to the face (blue arrow) is called *normal stress* or *axial stress*; the projection over the face (green arrow) is called *shear stress*. In turn, the shear stress is not necessarily parallel to one or another of the coordinate axes that define the plane of the face; thus, for each face the shear stress has in general two non-zero components (not shown in the figure).

[19] The vanishing of $\lim(\mathbf{M}/A)$ is qualitatively understood by observing that the distance to the center vanishes in the $A \to 0$ limit.

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It should be noted that the external action may also cause a rigid shift of the block because the latter is connected with the rest of the body (Fig. 2.8). Such a shift is not considered here because, as the block does not undergo a deformation, its potential energy does not change. To dispose of the shift one may assume that the prismatic block considered here is supplemented with a local reference, which also shifts as the external action is applied.

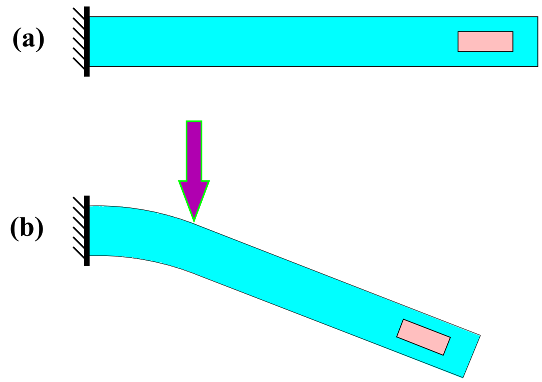

Fig. 2.8 Example of a situation in which the deformation of a larger body leaves the condition of an internal block unchanged. The larger body (the cyan area) is blocked at the left end, while the right end is unconstrained; **(a)** shows a situation where no force is acting, **(b)** shows the result of the application of a force (the vertical arrow) that bends the left part of the body. The potential energy of the smaller block (the pink area) is unaffected

2.14.1 Relations among the Stress Components

To identify possible relations among the stress components, one proceeds as follows. With reference to Fig. 2.7, consider first the two faces normal to the x_1 axis. For the right face, the normal unit vector pointing outward with respect to the block has the same direction as the unit vector $\mathbf{i}_1$ of the x_1 axis. The stress acting on this face will be indicated with $\mathbf{s}_1^+$, while that acting on the opposite face will be indicated with $\mathbf{s}_1^-$. The projections of $\mathbf{s}_1^+$ along the axes are given by the scalar products $\sigma_{1j}^+ = \mathbf{s}_1^+ \cdot \mathbf{i}_j$, with $j = 1,2,3$. The first one, σ_{11}^+, is normal to the face (*normal stress*); the other two projections, σ_{12}^+, σ_{13}^+, are parallel to the face (*shear stresses*). As for the opposite face, the components of $\mathbf{s}_1^-$ are found in the same manner. The force acting on each face is found by multiplying the stress ($\mathbf{s}_j^+$ or $\mathbf{s}_j^-$) by the area of the face; if the block is not subjected to accelerations along the axes, the forces acting on it must balance each other; this yields the vector relation

$$\left(\mathbf{s}_1^+ + \mathbf{s}_1^-\right) a_2\, a_3 + \left(\mathbf{s}_2^+ + \mathbf{s}_2^-\right) a_3\, a_1 + \left(\mathbf{s}_3^+ + \mathbf{s}_3^-\right) a_1\, a_2 = 0\,. \tag{2.112}$$

From the arbitrariness of the sides it follows that (2.112) is fulfilled if each term in parentheses vanishes independently; thus,

$$\mathbf{s}_j^+ = -\mathbf{s}_j^- , \qquad \sigma_{ij}^- = -\sigma_{ij}^+ . \tag{2.113}$$

This result is sketched in Fig. 2.9. The analysis shows that there is a total of 9

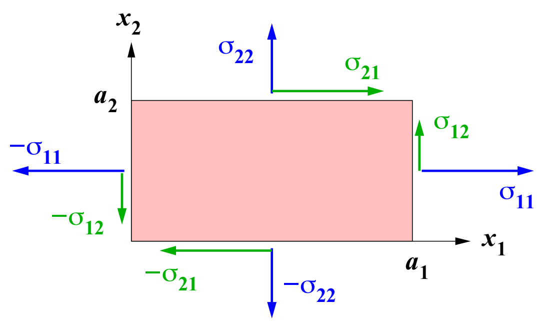

Fig. 2.9 Representation of the stress components relative to the faces normal to the x_1 and x_2 axes. If the block is not accelerating, the two pairs of normal stresses (blue arrows) balance each other, and, independently, the two pairs of shear stresses (green arrows) also balance each other. Other normal and shear stresses are present (not shown in the figure), that also balance pairwise

combinations of the stress indices, so that the stresses form a 3×3 tensor; however, the entries of such a tensor are not all independent. In fact, the fulfillment of (2.112) implies that the block does not accelerate along each axis, but does not prevent it from rotating around the center. Thus, additional relations are necessary to make the total torque exerted by the stress components to vanish. For this, it suffices to consider the shear stresses (Fig. 2.10), because the normal stresses, being applied to the center of each face, do not contribute to the torque. Considering the component

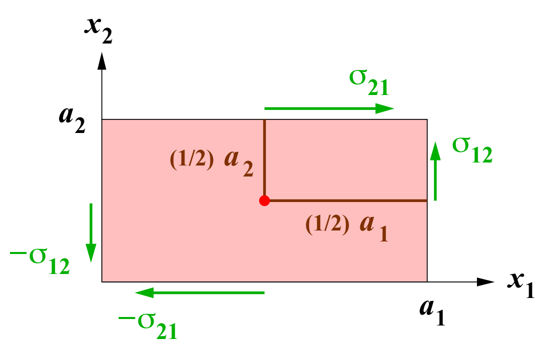

Fig. 2.10 Replica of Fig. 2.10 showing the calculation of the torque produced by the shear stresses (green arrows) around the centre (marked by the red dot) of the face normal to the x_3 axis. The distances from the rotational axis are in brown

of the torque around an axis parallel to x_3 and crossing the center of the block yields

$$\sigma_{12}\, a_2\, a_3\, \frac{a_1}{2} = \sigma_{21}\, a_3\, a_1\, \frac{a_2}{2} \qquad \Rightarrow \qquad \sigma_{21} = \sigma_{12} \, . \tag{2.114}$$

By the same token one finds $\sigma_{32} = \sigma_{23}$ and $\sigma_{13} = \sigma_{31}$, this showing that the stress tensor is symmetric.

2.15 Deformations

The discussion carried out in Sect. 2.14 has analyzed the equilibrium condition of a block of material subjected to surface forces, without taking into account the possibility of deformations produced by the forces themselves. To investigate this aspect, still with reference to the prismatic block of Fig. 2.7, consider the undeformed condition and select a point $\mathbf{r}$ of coordinates x_1, x_2, x_3 within the block. If the body is subjected to an external action that modifies its shape and/or position, the selected point shifts by a vector of coordinates ψ_1, ψ_2, ψ_3; each component ψ_i of the displacement depends on the external action and on the original position x_1, x_2, x_3.

To proceed, it is assumed that the surface forces applied to the block are such that the equilibrium condition holds, whence no acceleration of the block occurs; also, it is assumed that the deformations are small, so that a linear-response condition applies: since the displacements are small for each point x_1, x_2, x_3, their components can be approximated with a first-order expansion

Tensor

$$\psi_i(\mathbf{r}) = \psi_i(x_1,x_2,x_3) = \frac{\partial \psi_i}{\partial x_1} x_1 + \frac{\partial \psi_i}{\partial x_2} x_2 + \frac{\partial \psi_i}{\partial x_3} x_3 \,, \tag{2.115}$$

with $i = 1,2,3$. In (2.115), the coordinates are those of the chosen point in the undeformed situation, and the partial derivatives are calculated in the origin of the local reference. For the first-order expansion to hold it is necessary that the sides a_i of the block are small; also, (2.115) implies that one of the corners of the block coincides with the origin of the local reference, so that the displacement of such a corner is zero. It must be noted that the block may also be rigidly shifted due to the deformation of a larger body to which it belongs (compare with Fig. 2.8); the shift, however, is unimportant because it does not modify the potential energy of the block, and is made invisible in the calculations because it is compensated by the analogous shift of the local reference attached to one of the corners of the block.

The partial derivatives $\partial \psi_i / \partial x_j$ form a rank-2 tensor, which may be expressed as the sum of a symmetric and antisymmetric tensor:

$$\boxed{\frac{\partial \psi_i}{\partial x_j} = \frac{1}{2}\left(\frac{\partial \psi_i}{\partial x_j} + \frac{\partial \psi_j}{\partial x_i}\right) + \frac{1}{2}\left(\frac{\partial \psi_i}{\partial x_j} - \frac{\partial \psi_j}{\partial x_i}\right) .} \tag{2.116}$$

strain tensor

A comparison with (2.106) shows that the first term at the right hand side of (2.116) is the strain tensor ε_{ij}; in turn, the second term at the right hand side of (2.116) is an antisymmetric tensor whose entries will be indicated with

$$\theta_{ij} = \frac{1}{2}\left(\frac{\partial \psi_j}{\partial x_i} - \frac{\partial \psi_i}{\partial x_j}\right) . \tag{2.117}$$

Such a tensor has only three, non vanishing independent entries $\theta_{12}, \theta_{23}, \theta_{31}$; with the above definitions, the components of the displacement take the form

$$\begin{aligned}
\psi_1 &= \varepsilon_{11}x_1 + \varepsilon_{12}x_2 + \varepsilon_{13}x_3 + \theta_{31}x_3 - \theta_{12}x_2\,,\\
\psi_2 &= \varepsilon_{12}x_1 + \varepsilon_{22}x_2 + \varepsilon_{23}x_3 + \theta_{12}x_1 - \theta_{23}x_3\,,\\
\psi_3 &= \varepsilon_{13}x_1 + \varepsilon_{23}x_2 + \varepsilon_{33}x_3 + \theta_{23}x_2 - \theta_{31}x_1\,.
\end{aligned} \tag{2.118}$$

Changing the symbols as $\theta_{23} \leftarrow \theta_1$, $\theta_{31} \leftarrow \theta_2$, $\theta_{12} \leftarrow \theta_3$, and forming a vector $\mathbf{o} = (\theta_1, \theta_2, \theta_3)$, one finds that $\mathbf{o}$ is associated to the part of the displacement due to a rigid rotation; in fact, the terms of (2.118) involving the entries of $\mathbf{o}$ are the components of the vector product $\mathbf{o} \wedge \mathbf{r}$. On the other hand, a rigid rotation does not modify the potential energy of the block; as a consequence, the rotation may be disposed of by letting the local reference undergo such a rotation as well.[20] In conclusion, the remaining part of the displacement is that related to the local deformation of the body,[21]

This is related to Rotation

$$\begin{aligned}
\psi_1 &= \varepsilon_{11}x_1 + \varepsilon_{12}x_2 + \varepsilon_{13}x_3\,,\\
\psi_2 &= \varepsilon_{12}x_1 + \varepsilon_{22}x_2 + \varepsilon_{23}x_3\,,\\
\psi_3 &= \varepsilon_{13}x_1 + \varepsilon_{23}x_2 + \varepsilon_{33}x_3\,.
\end{aligned} \tag{2.119}$$

rotation terms are discarded because they don't affect the potential

The meaning of the strain tensor is readily explained by means of a few examples; to

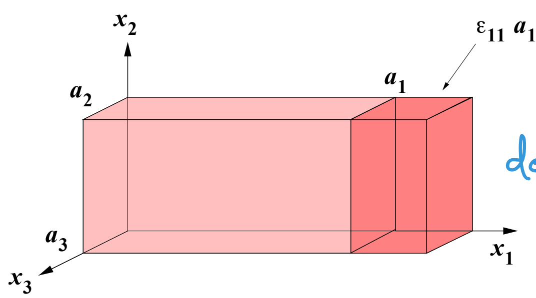

Fig. 2.11 Effect of a rigid shift ψ_1 of the face normal to the x_1 axis; as shown in the text, $\varepsilon_{11} = \psi_1/a_1$ is the relative shift with respect to the undeformed situation

deformation only along x_1?

proceed, it is convenient to assume that the sides a_i of the prismatic block are aligned with the corresponding axes x_i of the local reference, after the latter has undergone the translation and/or rotation due to the external action. As a first example, assume that all entries of the strain tensor are zero[22] with the exception of the normal stress ε_{11}; letting $x_1 = a_1$ in (2.119), one finds

deformation only along x_1

$$\psi_1(a_1, x_2, x_3) = \varepsilon_{11}\,a_1\,, \qquad \psi_2 = \psi_3 = 0\,. \tag{2.120}$$

---

[20] The reasoning is the same as that used earlier to dispose of the rigid shift.

[21] It is to be expected that the value of each entry of the strain tensor changes due to a rotation of the reference. The analysis of such changes is not considered here; in fact, it is identical to that relative to the stress tensor, carried out in Sect. 2.18.3.

[22] Due to the linearity of (2.119), one may consider one effect at the time and form their superposition at the end of the discussion; see, e.g., the reasoning that leads to the deformation shown in Fig. 2.14.

This shows that ε_{11} is the relative shift, with respect to the undeformed case, of the face of the block parallel to the $x_2 x_3$ plane (Fig. 2.11). The deformation is such that the face shifts without rotation, so that after the shift it is still parallel to the original plane; the same reasoning applies to the other diagonal entries. In conclusion, ε_{ii} provides the relative shift, with respect to the underformed case, along the x_i direction; for this reason, the diagonal entries of the strain tensor are called *extensions*.

As a second example, assume that all entries of the strain tensor are zero with the exception of the shear stress ε_{12}; letting $x_1 = a_1$, $x_2 = 0$ in (2.119), one finds

$$\psi_1 = 0, \qquad \psi_2(a_1, 0, x_3) = \varepsilon_{12}\, a_1 > 0, \qquad \psi_3 = 0, \tag{2.121}$$

that shows that the side connecting vertices $P = (a_1, 0, 0)$ and $Q = (a_1, 0, a_3)$ shifts by the amount $\psi_2 = \varepsilon_{12}\, a_1$ in the x_2 direction (Fig. 2.12). As a consequence, the face of the block originally coinciding with the $x_3 x_1$ plane rotates around the x_3 axis by the angle $\arctan(\varepsilon_{12}) \simeq \varepsilon_{12}$, where the approximation is due to the hypothesis of a small deformation ($\psi_2/a_1 \ll 1$). Similarly, letting $x_1 = 0$, $x_2 = a_3$ in (2.119), one

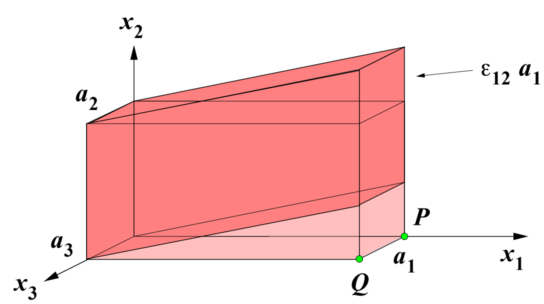

Fig. 2.12 Effect of the rotation around the x_3 axis of the face initially coinciding with the $x_3 x_1$ plane. The angle of rotation is $\arctan(\varepsilon_{12}) \simeq \varepsilon_{12}$; the result is the shift by $\varepsilon_{12}\, a_1$ of the PQ side and, consequently, of the right face of the block

finds

$$\psi_1(x_1, 0, a_3) = \varepsilon_{12}\, a_2 > 0, \qquad \psi_2 = \psi_3 = 0, \tag{2.122}$$

that shows that the side connecting vertices $(0, a_2, 0)$ and $(0, a_2, a_3)$ shifts by the amount $\varepsilon_{12}\, a_2$ in the x_1 direction. As a consequence, the face of the block originally coinciding with the $x_2 x_3$ plane rotates around the x_3 axis by the angle $\arctan(\varepsilon_{12}) \simeq \varepsilon_{12}$ (Fig. 2.13). If both rotations described by (2.121) and (2.122) occur, the two faces undergo a relative rotation by the angle $2\,\varepsilon_{12}$ (Fig. 2.14). The same results are found when examining the case $\varepsilon_{23} \neq 0$ or $\varepsilon_{31} \neq 0$. The non-diagonal entries of the strain tensor are called *shear strains* or *detrusions*.

2.16 Elasticity Law of a Continuous Medium

The preceding sections 2.14, 2.14.1, and 2.15 have introduced the concepts of stress, displacement, and strain from the macroscopic viewpoint, still assuming that the forces acting on the block of material under consideration balance each other.[23] Here, the case is considered where the forces do not balance, so that the relation (2.113) among the components of the stress tensor is not fulfilled any more, and the block is subjected to acceleration. Considering first the two faces normal to the x_1 axis, the umbalance of the stress components makes the sum $\sigma_{1j}^- + \sigma_{1j}^+$ to differ from zero; due to the smallness of the block one may assume, to first order,

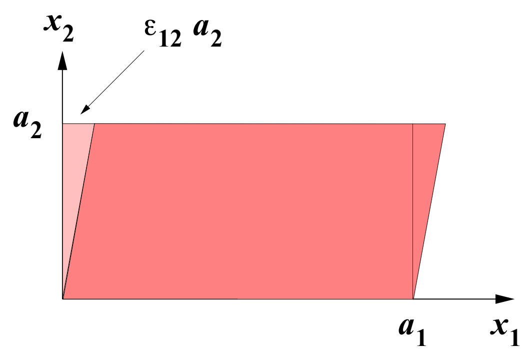

Fig. 2.13 Effect of a shear strain shifting the upper face of the block with respect of the lower face (lateral view). The face initially coinciding with the $x_2 x_3$ plane rotates by an angle $\arctan(\varepsilon_{12}) \simeq \varepsilon_{12}$.

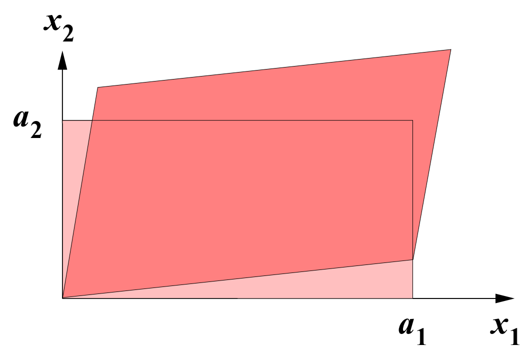

Fig. 2.14 Combination of the deformations shown in Figs. 2.12 and 2.13, described by (2.121) and (2.122), respectively (lateral view).

$$\sigma_{1j}^- + \sigma_{1j}^+ \simeq \frac{\partial \sigma_{1j}}{\partial x_1} a_1 , \qquad j = 1,2,3 , \tag{2.123}$$

where the partial derivative is supposed to be constant within the block. From (2.123) one readily calculates the unbalance in the jth component of the force:

$$\left(\sigma_{1j}^- + \sigma_{1j}^+\right) a_2 a_3 = \frac{\partial \sigma_{1j}}{\partial x_1} a_1 a_2 a_3 . \tag{2.124}$$

[23] Like in Sect. 2.14, gravity is not taken into account: the actions considered here derive from forces applied to the external surface of the block of material.

Adding up the contributions from the faces normal to the x_2 and x_3 axes yields for the jth component of the force acting over the block

$$\sum_{w=1}^{3} \frac{\partial \sigma_{wj}}{\partial x_w} a_1 a_2 a_3 = \sum_{w=1}^{3} \frac{\partial \sigma_{jw}}{\partial x_w} a_1 a_2 a_3 , \qquad j = 1,2,3 , \tag{2.125}$$

where the equality is due to the simmetry of the stress tensor. The jth component of the force equals the corresponding component of the acceleration $M\ddot{\psi}_j$, where ψ_j indicates a rigid displacement of the block along the j axis, and M is the mass of the block; as the latter is given by $M = \rho\, a_1 a_2 a_3$, with ρ the density of the material, replacing in (2.125) yields the elasticity law of a continuous medium:

$$\rho\, \ddot{\psi}_j = \sum_{w=1}^{3} \frac{\partial \sigma_{jw}}{\partial x_w} , \qquad j = 1,2,3 . \tag{2.126}$$

A comparison with (2.108) shows that (2.126), which has been derived basing on the unbalance of the forces acting on a continuous block of material, coincides with the law governing the dynamics of the nuclei for the acoustic modes in the long-wavelength limit. It is also interesting to note that the three quantities σ_{jw}, $w = 1,2,3$ that appear at the right hand side of (2.126) are the component of vector $\mathbf{s}$ defined in Sect. 2.14.1; therefore, (2.126) can be recast as

$$\rho\, \ddot{\psi}_j = \mathrm{div}(\mathbf{s}_j) , \qquad j = 1,2,3 . \tag{2.127}$$

2.17 The Cubic Crystal

The 9×9 elastic tensor Φ_{uw}^{ij} has been introduced in Sect. 2.12, where it has been shown that, basing on its definition (2.100) and exploiting the periodicity properties of the lattice, Φ_{uw}^{ij} is reduced to a 6×6 form without taking any other property of the crystal into account. Then, by exploiting the symmetry of the tensor, and still regardless of the type of the crystal, the number of independent entries is further reduced[24] from 36 to 21. In parallel, the symmetry of the stress and strain tensors is exploited as well, to reduce the number of independent entries of each of them from 9 to 6; then, after reordering the indices and renaming to $\mathbf{B}$ (*stiffness matrix*) the 6×6 form of the elastic tensor, the stress-strain relation has been recast in matrix form as (2.110). It is assumed that the stiffness matrix is nonsingular,[25] whence its inverse $\mathbf{H} = \mathbf{B}^{-1}$ (called *compliance matrix*) exists; both $\mathbf{B}$ and $\mathbf{H}$ are symmetric.[26]

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[24] As shown at p. 52, when the interatomic forces are of the central type, the number of independent entries reduces from 21 to 15.

[25] See also note 16 at p. 54.

[26] The stress-strain relation (2.110) derives from (2.107), namely, from a microscopic analysis of the long-wavelength limit of the acoustic modes. The same relation can be found from the

Depending on the crystal system, the number of independent entries of the elastic tensor is further reduced;[27] the minimum number of independent entries is three, that occurs in the cubic crystals. To demonstrate this, it is convenient to start (see also [30, App. A.3.1]) from the inverse relation of (2.110), that provides the strain vector as the product of the compliance matrix **H** times the stress vector. It is useful to remind that the first three entries of the strain vector, $\varepsilon_1 = \varepsilon_{11}, \dots$ are the normal strains, while the remaining three entries $\varepsilon_4 = \varepsilon_{23}, \dots$ are the shear strains; the same nomenclature applies to the stress vector. Remembering that **H** is symmetric, the expression of ε_4 reads

$$\varepsilon_4 = h_{11}\,\sigma_1 + h_{12}\,\sigma_2 + h_{13}\,\sigma_3 + h_{14}\,\sigma_4 + h_{15}\,\sigma_5 + h_{16}\,\sigma_6\,; \tag{2.128}$$

similar relations hold for ε_5 and ε_6. Assume that σ_1 is the only non-zero entry of the stress vector; the shear strains then become $\varepsilon_4 = h_{14}\,\sigma_1$, $\varepsilon_5 = h_{15}\,\sigma_1$, $\varepsilon_6 = h_{16}\,\sigma_1$; this, however, is impossible, because the application of σ_1 to a symmetric structure would produce an asymmetric deformation: a normal stress on the right face would in fact produce, among others, a shift of the upper face like that of Fig. 2.13. Such an outcome is prevented by letting $h_{14} = h_{15} = h_{16} = 0$. Repeating the reasoning starting from the condition where σ_2 or σ_3 is the only non-zero entry of the stress, yields $h_{24} = h_{25} = h_{26} = 0$ and, respectively, $h_{34} = h_{35} = h_{36} = 0$; in summary, the stress-strain relation becomes

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} = \begin{bmatrix} h_{11} & h_{12} & h_{13} & 0 & 0 & 0 \\ h_{12} & h_{22} & h_{23} & 0 & 0 & 0 \\ h_{13} & h_{23} & h_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & h_{44} & h_{45} & h_{46} \\ 0 & 0 & 0 & h_{45} & h_{55} & h_{56} \\ 0 & 0 & 0 & h_{46} & h_{56} & h_{66} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} . \tag{2.129}$$

Next, assume that σ_5 is the only non-zero entry of the stress vector; the shear strains then become $\varepsilon_4 = h_{45}\,\sigma_5$, $\varepsilon_5 = h_{55}\,\sigma_5$, $\varepsilon_6 = h_{56}\,\sigma_5$; the first and third of the above must be zero to prevent another type of asymmetric deformation from occurring: therefore, it must be $h_{45} = h_{56} = 0$. Repeating the reasoning after assuming that σ_4 is the only non-zero entry of the stress vector yields $h_{46} = 0$; in summary, the 3×3 lower-right part of **H** reduces to the diagonal form.

Coming now to the first line of the 3×3 upper-left part of **H**, one may consider (for any value of σ_{11}) the situation where $\sigma_{22} \neq 0$, $\sigma_{33} = 0$ and the other situation where $\sigma_{22} = 0$, $\sigma_{33} \neq 0$; since the two situations correspond to exchanging the x_2 and x_3 axes, which in a cubic crystal has no effect, the strain ε_{11} must remain the same: this implies $h_{13} = h_{12}$. Similarly, in the second line one takes the situations $\sigma_{33} \neq 0$, $\sigma_{11} = 0$ and $\sigma_{33} = 0$, $\sigma_{11} \neq 0$, to find $h_{23} = h_{12}$; in conclusion, all non-diagonal entries of the 3×3 upper-left part of **H** have the same value, say, h_{12}.

macroscopic analysis started in Sect. 2.14: for this, one introduces the strain and stress tensors, and assumes that the linear-response condition applies.

[27] A list of the possible cases is given, e.g., in [1, Tab. 22.1]).

The analysis is concluded by observing that, again due to the symmetry of the cubic crystal, any permutation of the coordinate axes has no effect on the normal strains nor, separately, on the shear strains; as a consequence, the diagonal entries of the upper-left part of **H** must be equal to each other; by the same token, the diagonal entries of the lower-right part of **H** must be equal to each other. In conclusion, the stress-strain relation of a cubic crystal becomes

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} = \begin{bmatrix} h_{11} & h_{12} & h_{12} & 0 & 0 & 0 \\ h_{12} & h_{11} & h_{12} & 0 & 0 & 0 \\ h_{12} & h_{12} & h_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & h_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & h_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & h_{44} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix}; \tag{2.130}$$

as anticipated, the number of independent entries reduces to three. The stiffness matrix $\mathbf{B} = \mathbf{H}^{-1}$ reads (the calculation is carried out in Prob. 2.9):

$$\mathbf{B} = \begin{bmatrix} b_{11} & b_{12} & b_{12} & 0 & 0 & 0 \\ b_{12} & b_{11} & b_{12} & 0 & 0 & 0 \\ b_{12} & b_{12} & b_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/h_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/h_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/h_{44} \end{bmatrix}, \tag{2.131}$$

with

$$b_{11} = \frac{h_{11} + h_{12}}{(h_{11} - h_{12})(h_{11} + 2h_{12})}, \qquad b_{12} = \frac{-h_{12}}{(h_{11} - h_{12})(h_{11} + 2h_{12})}, \tag{2.132}$$

showing that **B** is symmetric (as expected, see Prob. 2.8) and has the same structure as **H**. The opposite procedure, starting from **B** to calculate **H**, provides the entries h_{ij} in terms of b_{ij}; letting $D_b = (b_{11} - b_{12})(b_{11} + 2b_{12})$,

$$h_{11} = \frac{b_{11} + b_{12}}{D_b}, \qquad h_{12} = -\frac{b_{12}}{D_b}, \qquad h_{44} = \frac{1}{b_{44}}. \tag{2.133}$$

The compliance and stiffness matrices are used also in problems typical of structural engineering; the symbols used in that context, however, are different: considering for instance a situation in which only one normal stress, say, σ_1, is present, the corresponding normal strain reads

$$\varepsilon_1 = h_{11}\,\sigma_1 = \frac{1}{E}\,\sigma_1, \tag{2.134}$$

with E the *Young modulus*. Still in the case when only σ_1 is present, one derives from (2.130) the normal strains in the other two directions,

$$\varepsilon_2 = \varepsilon_3 = h_{12}\,\sigma_1 = \frac{h_{12}}{h_{11}}\,h_{11}\,\sigma_1 = -\frac{\nu}{E}\,\sigma_1\,, \qquad \nu = -\frac{h_{12}}{h_{11}} > 0\,, \tag{2.135}$$

with ν the *Poisson coefficient*. The reason for the negative sign is readily understood on physical grounds: if σ_1 is such that the material stretches in the x_1 direction, the block typically shrinks in the other two directions (like in the example of Fig. 2.15);[28] conversely, if the material is compressed in the x_1 direction, it swells in the other two directions.[29] From (2.135) one also derives $\varepsilon_2 = -\nu\,\varepsilon_1$. Definitions

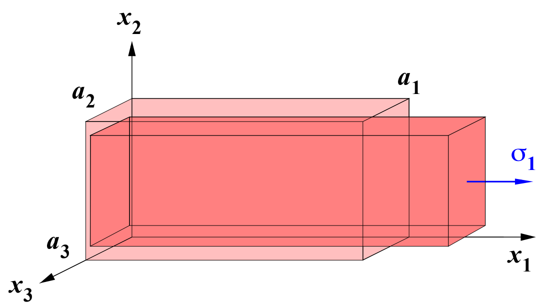

Fig. 2.15 A prismatic block of material of sides a_1, a_2, a_3, whose left face is kept fixed while the right face is subjected to a tensile normal stress (blue arrow). The block stretches in the x_1 direction and shrinks in the x_2 and x_3 directions according to (2.134, 2.135).

(2.134) and (2.135) show that E has the units of a tension while ν is dimensionless. If all normal stresses are simultaneously present, $\sigma_1, \sigma_2, \sigma_3 \neq 0$, the effects linearly combine to yield

$$\varepsilon_1 = \frac{\sigma_1 - \nu\,(\sigma_2 + \sigma_3)}{E}\,, \quad \varepsilon_2 = \frac{\sigma_2 - \nu\,(\sigma_3 + \sigma_1)}{E}\,, \quad \varepsilon_3 = \frac{\sigma_3 - \nu\,(\sigma_1 + \sigma_2)}{E}\,. \tag{2.136}$$

Considering now the shear stresses, from (2.130) one finds

$$\varepsilon_i = h_{44}\,\sigma_i = \frac{1}{G}\,\sigma_i\,, \qquad i = 4,5,6\,, \tag{2.137}$$

with $G = 1/h_{44}$ the *shear modulus*, whose units are those of a tension. Using the new symbols, (2.130) becomes

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} = \begin{bmatrix} 1/E & -\nu/E & -\nu/E & 0 & 0 & 0 \\ -\nu/E & 1/E & -\nu/E & 0 & 0 & 0 \\ -\nu/E & -\nu/E & 1/E & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/G \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix}; \tag{2.138}$$

[28] Fig. 2.15 seems to contradict Fig. 2.11, in which no shrinking in the x_2 or x_3 directions appears. In fact, Fig. 2.11 was derived in the hypothesis that all entries of the strain tensor could be fixed independently; the analysis shown here indicates that this is not the case.

[29] It is interesting to note that there are materials, called *auxetics*, having a negative Poisson coefficient. When stretched, they become thicker in the transversal directions.

from (2.132) one also derives

$$b_{11} = \frac{(1-\nu)\,E}{(1+\nu)\,(1-2\,\nu)}\,, \quad b_{12} = \frac{\nu\,E}{(1+\nu)\,(1-2\,\nu)}\,, \quad b_{44} = G\,. \tag{2.139}$$

2.17.1 The Isotropic Material

The description of the compliance matrix of a cubic crystal, carried out above, has derived a number of relations among the entries of the matrix, due to the inherent symmetries of the crystal. The same relations among the entries apply also to the stiffness matrix; the end result is that these matrices have only three independent entries, as shown in (2.130) and (2.131).

When an isotropic material is considered, it is possible to demonstrate that the structure of the compliance and stiffness matrices remains the same, whereas the number of independent entries reduces to two;[30] considering for instance the stiffness matrix, the following relation among the entries is found:

$$b_{11} = b_{12} + 2\,b_{44}\,. \tag{2.140}$$

From (2.139) it follows

$$E = 2\,G\,(1+\nu)\,. \tag{2.141}$$

2.18 Complements

2.18.1 The Bloch Theorem in the Discrete Case

Let $z_k(\mathbf{r})$ be the kth component of a position-dependent vector. A *translation operator* $\mathscr{T}_i = \mathscr{T}(\mathbf{l}_i)$ associated to the ith vector $\mathbf{l}_i$ of the direct lattice is defined by the property

$$\mathscr{T}_i\, z_k(\mathbf{r}) = z_k(\mathbf{r} + \mathbf{l}_i) \tag{2.142}$$

for any $z_k(\mathbf{r})$. Translation operators are commutative:

$$\mathscr{T}_i\, \mathscr{T}_s\, z_k(\mathbf{r}) = z_k(\mathbf{r} + \mathbf{l}_i + \mathbf{l}_s) = \mathscr{T}_s\, \mathscr{T}_i\, z_k(\mathbf{r})\,; \tag{2.143}$$

therefore, all translation operators have a common set of eigenfunctions v. The form of the latter, and of the corresponding eigenvalues α, can be worked out from (2.142, 2.143); in fact, given three arbitrary vectors $\mathbf{l}_i$, $\mathbf{l}_s$, $\mathbf{l}_u$, the eigenvalue equations generated by the corresponding translation operators are

[30] See, e.g., [59, Sects. 60, 61]. The property is demonstrated by prescribing the invariance of the elastic tensor under an infinitesimal rotation of the coordinates.

$$\mathscr{T}_i\, v = \alpha(\mathbf{l}_i)\, v\,, \qquad \mathscr{T}_s\, v = \alpha(\mathbf{l}_s)\, v\,, \qquad \mathscr{T}_u\, v = \alpha(\mathbf{l}_u)\, v\,. \tag{2.144}$$

Combining the first two relations in (2.144) yield $\mathscr{T}_i\,\mathscr{T}_s\, v = \mathscr{T}_i\,\alpha(\mathbf{l}_s)\, v = \alpha(\mathbf{l}_i)\,\alpha(\mathbf{l}_s)\, v$. Thanks to the arbitrariness of the vectors, one may let $\mathbf{l}_u = \mathbf{l}_i + \mathbf{l}_s$, to find $\mathscr{T}_i\,\mathscr{T}_s\, v(\mathbf{r}) = v(\mathbf{r} + \mathbf{l}_i + \mathbf{l}_s) = \mathscr{T}_u\, v(\mathbf{r})$, whence[31] $\mathscr{T}_u = \mathscr{T}_i\,\mathscr{T}_s$. Using the latter with the third relation in (2.144) provides

$$\alpha(\mathbf{l}_i)\,\alpha(\mathbf{l}_s) = \alpha(\mathbf{l}_u) = \alpha(\mathbf{l}_i + \mathbf{l}_s)\,. \tag{2.145}$$

This result shows that the functional dependence of α on the translation vector must be of the exponential type,

$$\alpha(\mathbf{l}_i) = \exp(\mathbf{c} \cdot \mathbf{l}_i)\,, \tag{2.146}$$

with $\mathbf{c}$ given by (2.59). Combining the eigenfunction equation (2.144) with definition (2.142), to find $\mathscr{T}_i\, v(\mathbf{r}) = \alpha(\mathbf{l}_i)\, v(\mathbf{r}) = v(\mathbf{r} + \mathbf{l}_i)$, and using the form (2.146) of the eigenvalue, yields the *Bloch theorem (first form)*:

$$v_{\mathbf{c}}(\mathbf{r} + \mathbf{l}_i) = \exp(\mathbf{c} \cdot \mathbf{l}_i)\, v_{\mathbf{c}}(\mathbf{r})\,, \tag{2.147}$$

where the index reminds one that the eigenfunction depends on the choice of $\mathbf{c}$. A special form of (2.147) is found by letting $\mathbf{r} = 0$:

$$v_{\mathbf{c}}(\mathbf{l}_i) = \exp(\mathbf{c} \cdot \mathbf{l}_i)\, v_{\mathbf{c}}(0)\,. \tag{2.148}$$

An alternative form of (2.147) is found by introducing the auxiliary function $u_{\mathbf{c}}(\mathbf{r}) = v_{\mathbf{c}}(\mathbf{r})\, \exp(-\mathbf{c} \cdot \mathbf{r})$, so that (2.147) becomes

$$v_{\mathbf{c}}(\mathbf{r} + \mathbf{l}_i) = \exp(\mathbf{c} \cdot \mathbf{l}_i)\, u_{\mathbf{c}}(\mathbf{r})\, \exp(\mathbf{c} \cdot \mathbf{r})\,; \tag{2.149}$$

in turn, from the definition of $u_{\mathbf{c}}$ one finds $v_{\mathbf{c}}(\mathbf{r} + \mathbf{l}_i) = u_{\mathbf{c}}(\mathbf{r} + \mathbf{l}_i)\, \exp[\mathbf{c} \cdot (\mathbf{r} + \mathbf{l}_i)]$; combining the latter with (2.149) yields the *Bloch theorem (second form)*:

$$v_{\mathbf{c}}(\mathbf{r}) = u_{\mathbf{c}}(\mathbf{r})\, \exp(\mathbf{c} \cdot \mathbf{r})\,, \qquad u_{\mathbf{c}}(\mathbf{r} + \mathbf{l}_i) = u_{\mathbf{c}}(\mathbf{r})\,. \tag{2.150}$$

The derivations of this section still hold true if the generic position vector $\mathbf{r}$ is replaced with a lattice vector $\mathbf{l}_k$; in this case, for instance, (2.142) becomes

$$\mathscr{T}_i\, z_k(\mathbf{l}_k) = z_k(\mathbf{l}_k + \mathbf{l}_i) \tag{2.151}$$

Given this premise, one may apply a translation operator to the left hand side of (2.56), to obtain

$$\mathscr{T}_i \sum_{n\beta w} d_{\alpha u}^{\beta w}(\mathbf{l}_m - \mathbf{l}_n)\; z_{\beta w}(\mathbf{l}_n) = \sum_{n\beta w} d_{\alpha u}^{\beta w}(\mathbf{l}_m - \mathbf{l}_n)\; z_{\beta w}(\mathbf{l}_n + \mathbf{l}_i) =$$

$$= \sum_{n\beta w} d_{\alpha u}^{\beta w}(\mathbf{l}_m - \mathbf{l}_n)\;\; \mathscr{T}_i\, z_{\beta w}(\mathbf{l}_n)\,, \tag{2.152}$$

[31] It is easily found that the relation $\mathscr{T}_u = \mathscr{T}_i\,\mathscr{T}_s$ holds not only for the eigenfunctions $v(\mathbf{r})$ but for any function $z_k(\mathbf{r})$.

where the entry of the dynamic matrix is unaffected because $(\mathbf{l}_m + \mathbf{l}_i) - (\mathbf{l}_n + \mathbf{l}_i) = \mathbf{l}_m - \mathbf{l}_n$. This shows that the dependence of the dynamic matrix on the translation vectors of the lattice is such, that the matrix commutes with any $\mathscr{T}_i$. As a consequence, the solutions $z_{\alpha u}(\mathbf{l}_m)$ of (2.56) are also eigenfunctions of the translation operators; namely, comparing with (2.148), they have the form (2.58).

2.18.2 Components of Vectors and Tensors

To express vectors and tensors in terms of their components with respect to a given reference, one can consider the tetrahedral block of material shown in Fig. 2.16. Let A be the area of the PQR face, and A_2 the area of the POR face; the former one, PQR, can be thought of as originating from a rotation of POR around the PR line, in which vertex O shifts along the x_2 axis to reach point Q; as a consequence it is $A_2 = A\cos(\varphi_2)$, where φ_2 is the angle between OL and QL, with OL the normal drawn from the origin to line PR. If $\mathbf{i}_1$, $\mathbf{i}_2$, $\mathbf{i}_3$ are the unit vectors of the axes, and $\mathbf{n}$ is the unit vector normal to face PQR, then[32] it is $\cos(\varphi_2) = \mathbf{n}\cdot\mathbf{i}_2$. By the same token one concludes

$$A_i = A\cos(\varphi_i), \qquad \cos(\varphi_i) = \mathbf{n}\cdot\mathbf{i}_i, \qquad i = 1,2,3. \tag{2.153}$$

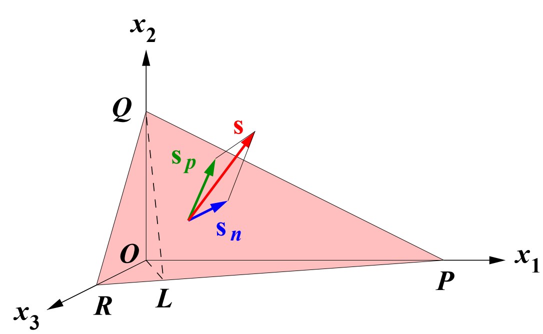

Fig. 2.16 A tetrahedral block of material. The red arrow shows the stress $\mathbf{s} = \lim_{A\to 0}\mathbf{F}/A$, with A the area of the PQR face. The blue arrow is the projection of the stress along the direction normal to the face, while the green arrow is the projection over the face. The same structure of vectors (not drawn in the figure) applies to all remaining faces

Still with reference to Fig. 2.16, let $\mathbf{s}$ be the stress acting on the PQR face; the stresses acting on the other three faces (not shown in the figure) are indicated here with $\mathbf{t}_1$, $\mathbf{t}_2$, $\mathbf{t}_3$, respectively for the face normal to axis x_1, x_2, and x_3. The equilibrium condition for the block is[33] $\mathbf{s}\,A = \mathbf{t}_1 A_1 + \mathbf{t}_2 A_2 + \mathbf{t}_3 A_3$ or, dividing both sides by A,

[32] In fact, $\mathbf{n}$ is normal to QL and $\mathbf{i}_2$ is normal to OL.

[33] Volume forces may also be present; however, in the limit where the block becomes very small, they tend to higher-order infinitesimals with respect to the surface forces (see also the note at p. 56).

$$\mathbf{s} = e_1\,\mathbf{t}_1 + e_2\,\mathbf{t}_2 + e_3\,\mathbf{t}_3\,, \qquad e_i = \cos(\varphi_i)\,. \tag{2.154}$$

In turn, each stress $\mathbf{t}_i$ can be projected on the coordinate axes to yield[34] the components $\sigma_{ij} = \mathbf{t}_i \cdot \mathbf{i}_j$; from this, one expresses the components of $\mathbf{s}$ in the $x_1\,x_2\,x_3$ reference as

$$s_j = \mathbf{s}\cdot\mathbf{i}_j = e_1\,\mathbf{t}_1\cdot\mathbf{i}_j + e_2\,\mathbf{t}_2\cdot\mathbf{i}_j + e_3\,\mathbf{t}_3\cdot\mathbf{i}_j = e_1\,\sigma_{1j} + e_2\,\sigma_{2j} + e_3\,\sigma_{3j}\,. \tag{2.155}$$

A representation of the form (2.155), based on the projections of $\mathbf{s}$ onto the coordinate axes, is called *extrinsic*. Another representation, called *intrinsic*, is based on the projections of $\mathbf{s}$ on the normal $\mathbf{n}$ to the face and on the plane of the face. Referring to Fig. 2.16 and using (2.154) provides, for the projection on the normal,

$$s_n = \mathbf{s}\cdot\mathbf{n} = \mathbf{n}\cdot(e_1\,\mathbf{t}_1 + e_2\,\mathbf{t}_2 + e_3\,\mathbf{t}_3)\,. \tag{2.156}$$

On the other hand, projecting $\mathbf{n}$ on the coordinate axes, and using the second relation in (2.153) along with the short-hand notation $e_i = \cos(\varphi_i)$, yields

$$\mathbf{n} = (\mathbf{n}\cdot\mathbf{i}_1)\;\mathbf{i}_1 + (\mathbf{n}\cdot\mathbf{i}_2)\;\mathbf{i}_2 + (\mathbf{n}\cdot\mathbf{i}_3)\;\mathbf{i}_3 = e_1\,\mathbf{i}_1 + e_2\,\mathbf{i}_2 + e_3\,\mathbf{i}_3\,. \tag{2.157}$$

Replacing (2.157) in (2.156), and remembering that $\sigma_{ij} = \mathbf{t}_i\cdot\mathbf{i}_j$, provides

$$s_n = (e_1\,\mathbf{i}_1 + e_2\,\mathbf{i}_2 + e_3\,\mathbf{i}_3)\cdot(e_1\,\mathbf{t}_1 + e_2\,\mathbf{t}_2 + e_3\,\mathbf{t}_3) = \sum_{ij}\sigma_{ij}\,e_i\,e_j\,, \tag{2.158}$$

expressing the normal stress s_n in terms of the components of the stress tensor and of the angles between the normal $\mathbf{n}$ to the face and each of the coordinate axes. As for the component s_b on the PQR plane (Fig. 2.16), one considers the line along which the PQR plane is intercepted by the plane formed by $\mathbf{s}$ and $\mathbf{n}$; the expression of the s_b component is found by projecting $\mathbf{s}$ on the unit vector $\mathbf{b}$ of such a line. Its structure is similar to that of (2.158) and reads

$$s_b = \sum_{ij}\sigma_{ij}\,e_i\,f_j\,, \tag{2.159}$$

with $f_i = \mathbf{b}\cdot\mathbf{i}_i$. The derivation of (2.159) is shown in Prob. 2.10; the general expression for the transformation of the components of a rank-2 tensor under a reference rotation is derived in Sect. A.4.

2.18.3 Principal Stresses

It has been shown in Sect. 2.18.2 that the stress normal to a face can be expressed as in (2.158), namely,

[34] Here and in the next section it is convenient to use the two-index notation for the stress tensor instead of the single-index notation introduced with (2.109).

$$s_n = \sigma_{11}\, e_1^2 + \sigma_{22}\, e_2^2 + \sigma_{33}\, e_3^2 + 2\,\sigma_{23}\, e_2\, e_3 + 2\,\sigma_{31}\, e_3\, e_1 + 2\,\sigma_{12}\, e_1\, e_1\,. \qquad (2.160)$$

Considering the tetrahedral block of Fig. 2.16, assume that points P, Q, and R are shifted, independently from each other, along the x_1, x_2, and x_3 axes, respectively. These shifts modify the orientation of the PQR face, without affecting the orientations of the other three faces of the block. As a consequence, the direction of $\mathbf{n}$, hence the values of e_1, e_2, e_3, are changed, whereas the entries σ_{ij} of the stress tensor are left unmodified. From this viewpoint, one may consider s_n in (2.160) as a quadratic form in the e_i variables, whose coefficients σ_{ij} are prescribed.

It is of interest to determine whether values of e_i exist, that make s_n to attain an extremum. For this, one could think of calculating the derivatives $\partial s_n/\partial e_i$ and putting them equal to zero; this procedure, however, would not be correct because the e_i variables are not independent from each other: in fact, due to definition (2.154), they fulfill the constraint $e_1^2 + e_2^2 + e_3^2 = 1$. The correct calculation consists therefore in determining a constrained extremum, using a Lagrange multiplier λ (see, e.g., [50, Sect. B.6]). Letting $F_e = 1 - (e_1^2 + e_2^2 + e_3^2)$, so that the constraint becomes $F_e = 0$, one constructs the function

$$F = \sigma_{11}\, e_1^2 + \sigma_{22}\, e_2^2 + \sigma_{33}\, e_3^2 + 2\,\sigma_{23}\, e_2\, e_3 + 2\,\sigma_{31}\, e_3\, e_1 + 2\,\sigma_{12}\, e_1\, e_2 + \lambda\, F_e\,. \qquad (2.161)$$

Equating to zero the derivatives $\partial F/\partial e_i$ one finds the a system of three linear, homogeneous equations

$$\begin{aligned} \sigma_{11}\, e_1 + \sigma_{12}\, e_2 + \sigma_{31}\, e_3 &= \lambda\, e_1\,, \\ \sigma_{12}\, e_1 + \sigma_{22}\, e_2 + \sigma_{23}\, e_3 &= \lambda\, e_2\,, \\ \sigma_{13}\, e_1 + \sigma_{23}\, e_2 + \sigma_{33}\, e_3 &= \lambda\, e_3\,. \end{aligned} \qquad (2.162)$$

In conclusion, the problem of finding the orientation of the PQR face that makes σ_n stationary is equivalent to finding the three eigenvalues λ_1, λ_2, λ_3 of the stress tensor. The eigenvalues are found by solving the algebraic equation[35]

$$\det \begin{bmatrix} \sigma_{11} - \lambda & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} - \lambda & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} - \lambda \end{bmatrix} = 0\,, \qquad (2.163)$$

and are real because the stress tensor is symmetric.[36] Inserting λ_1 into the algebraic system one finds the values of e_1, e_2, e_3 corresponding to it; such values are the components of the first eigenvector $\mathbf{v}_1$. Then, one proceeds in a similar way with λ_2 and λ_3; in summary,

---

[35] Eq. (2.163) is also called *secular equation*. The term is due to Laplace (1749–1827), who introduced the equation while investigating planetary motions.

[36] See, e.g., the demonstration in Prob. 2.5.

$$\lambda_1 \to \mathbf{v}_1 = \begin{bmatrix} v_{11} \\ v_{12} \\ v_{13} \end{bmatrix}, \qquad \lambda_2 \to \mathbf{v}_2 = \begin{bmatrix} v_{21} \\ v_{22} \\ v_{23} \end{bmatrix}, \qquad \lambda_3 \to \mathbf{v}_3 = \begin{bmatrix} v_{31} \\ v_{32} \\ v_{33} \end{bmatrix}. \tag{2.164}$$

As the eigenvalues and all coefficients of the algebraic system are real, the eigenvectors are real as well; also, due to the homogeneity of the algebraic system (2.162), the eigenvectors are defined apart from a multiplicative factor, whence they can be normalized to unity. Due to the symmetry of the stress tensor, if the eigenvalues are different from each other, then the eigenvectors are mutually orthogonal; if there are multiple eigenvalues, it is in any case possible to find three mutually-orthonormal eigenvectors [50, Sect. A.11.2]: in conclusion, one has

$$\mathbf{v}_s \cdot \mathbf{v}_r = \delta_{rs}, \tag{2.165}$$

with δ_{rs} the Kronecker symbol (A.1). It follows that the 3×3 matrix $\mathbf{V}$ whose first, second, and third columns are equal, respectively, to $\mathbf{v}_1$, $\mathbf{v}_2$, and $\mathbf{v}_3$ is orthogonal, namely (Sect. A.2), $\mathbf{V}^T = \mathbf{V}^{-1}$. As the nine entries of $\mathbf{V}$ are connected to each other by the six relations (2.165), only three of them are independent (see the analogous comment in A.2). Due to the normalization, the individual components of the eigenvectors can also be expressed as

$$v_{rk} = \mathbf{v}_r \cdot \mathbf{i}_k = \cos(\gamma_{rk}), \tag{2.166}$$

with $\mathbf{i}_k$ the unit vector of the kth axis and γ_{rk} the angle between $\mathbf{v}_r$ and $\mathbf{i}_k$ (compare with (A.12)).

It is of interest to check the effect of the transformation produced by $\mathbf{V}$ upon the stress tensor; for this, letting σ'_{ij} be the entries of the transformed stress tensor, one applies the general transformation (A.24) to find

$$\sigma'_{ij} = \sum_{rs} \sigma_{rs}\, v_{ir}\, v_{js} = \sum_r v_{ir} \sum_s \sigma_{rs}\, v_{js}. \tag{2.167}$$

Thanks to the eigenvalue equation (2.162) it is

$$\sum_s \sigma_{rs}\, v_{js} = \lambda_j\, v_{jr}, \qquad \sigma'_{ij} = \sum_r v_{ir}\, \lambda_j\, v_{jr} = \lambda_j\, \delta_{ij} \tag{2.168}$$

or, in matrix form,

$$\begin{bmatrix} \sigma'_{11} & \sigma'_{12} & \sigma'_{13} \\ \sigma'_{21} & \sigma'_{22} & \sigma'_{23} \\ \sigma'_{31} & \sigma'_{32} & \sigma'_{33} \end{bmatrix} = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}. \tag{2.169}$$

In conclusion, at any point it is always possible to find three orthogonal directions such as, along each direction, the normal stress takes a stationary value and the shear stress is absent, i.e., the stress tensor is diagonal. Such directions are called *principal axes*, and the corresponding components λ_1, λ_2, λ_3 are the *principal stresses*; the coordinate planes determined by the principal axes are called *principal planes*. If the three principal stresses are different, the principal axes are uniquely determined; if two principal stresses are equal, say, $\lambda_2 = \lambda_3$, then an infinite number of principal references exists: specifically, such references are those having $\mathbf{v}_1$ as the first unit vector, while $\mathbf{v}_2$ and $\mathbf{v}_3$ are mutually-orthogonal unit vectors arbitrarily chosen within the plane normal to $\mathbf{v}_1$. Finally, if all principal stresses are equal, any orthogonal reference is principal.

If the three principal stresses $\lambda_1, \lambda_2, \lambda_3$ differ from zero, the stress condition is called *triaxial*; if only two of them differ from zero, the stress condition is called *biaxial* or *planar*; finally, if only one principal stress differs from zero, the stress condition is called *uniaxial*.

Continuation of lecture in Mechanical

Advanced Solid-State Sensors M

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Course Program 2019-2020

Mechanical Sensors

Characterization of mechanical sensors

- the measurand and the physical structures

  1. Most relevant mechanical signals, their units in the S.I., and ranges for specific applications
  2. Definition of the stress and strain tensors
  3. Description of the structural elements mainly used in solid-state sensors (beams & plates)

List of mechanical measurands:

subset of six signals covering the most important classes of mechanical microsensors

- Pressure/Stress
- Acceleration/Deceleration
- Displacement
- Flow rate
- Force/Torque
- Position/Angle

Automotive accelerometers

Application	Range Gravitational Acceleration
Frontal airbags	+/- 50 g
Lateral airbags	+/- 100 – 250 g
Suspensions	+/- 2 g
ABS (Antilock Braking System)	+/- 1 g

Units are referred to g, with $g = 9{,}8\ m/s^2$

Pressure units (Pascal)

1 Pa	International System
1 KPa	1e3 Pa
1 kgf/m^2	9,8 Pa (g = 9,8 m/s^2)
1 psi (pound-force per square inch)	6,89e3 Pa (1inch = 25.4mm; 1Kg = 2,2046p)
1 mmHg (= 1 Torr)	1,33e2 Pa density of mercury (ρ_{Hg} = 13,59 g/cm^3, liquid)
1 atm	760 Torr = 1,01e5 Pa (equivalent to 10,33 m of water)
1 bar	1e5 Pa

Applications of silicon pressure sensors

Application	Pressure Range
Manifold pressure	15 - 250 kPa
Fuel pressure	15 - 400 kPa
Tyre pressure	1,8 –2,5 bar
Blood pressure (max 120 – 130 mmHg; min 70 – 80 mmHg)	30 - 300 mmHg
Barometric pressure	in hectopascal = mbar o in mmHg

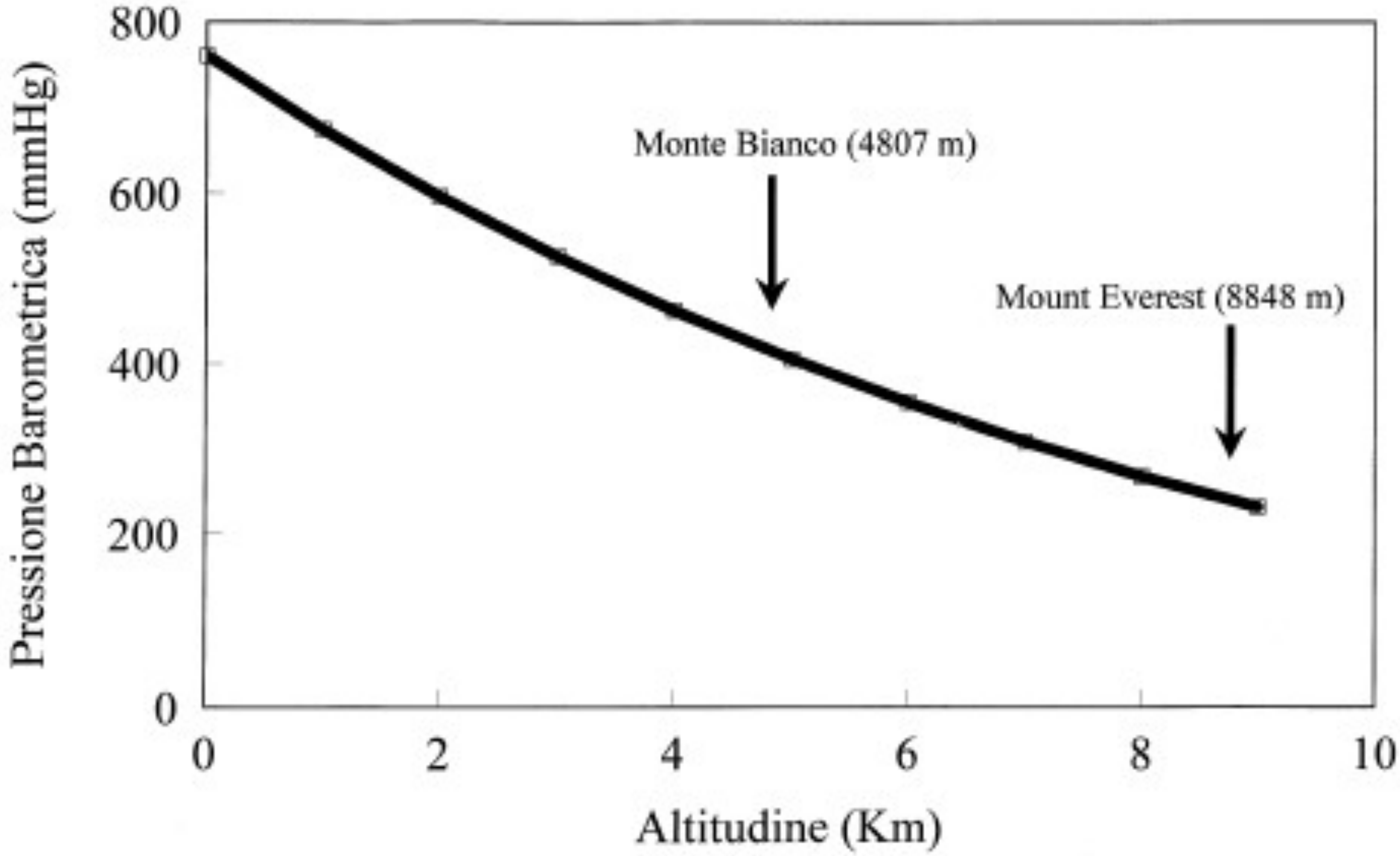

Figura 1. *Modificazione della pressione barometrica in relazione all'altitudine secondo le tabelle dell'Organizzazione dell'Aviazione Civile Internazionale.*

Mechanical Sensors

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1. Most relevant mechanical signals, their units in the S.I., and ranges for specific applications
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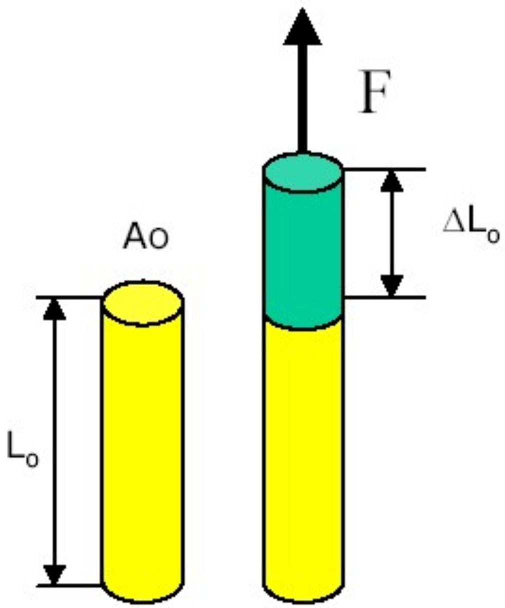
Definition of stress and strain tensors



Stress: $\sigma = F/A_0$ [Pa = N/m^2]

Strain: $\varepsilon = \Delta L_0/L_0$

HOOKE's LAW:

$E = \sigma / \varepsilon$ Young's modulus [Pa]

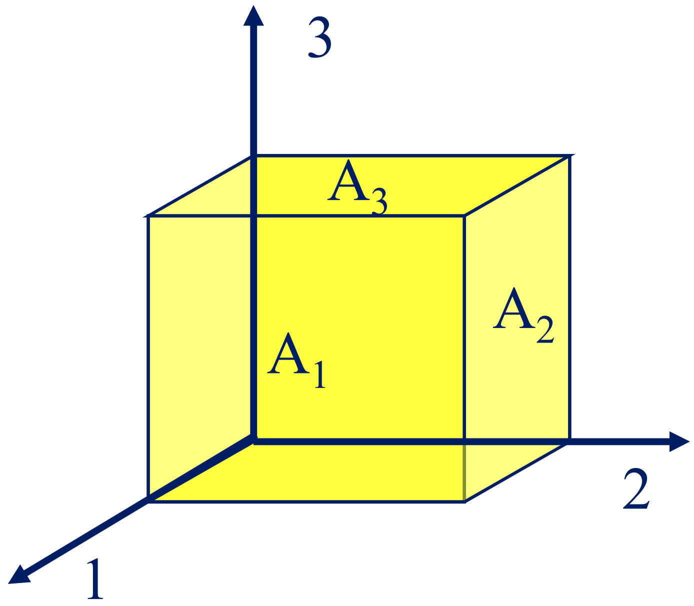
Assumptions

- We will consider elastic deformations and linear response → small-deformation hypotesis.
- In equilibrium, the resultant force over the body is 0, the resultant moment over the body is 0.
- The linear dimensions of the physical system are large enough to consider it as a continuous body (example: lattice distance in silicon a=5,431 Å, MEMS structures with $L_{min} \approx 50$ nm).
- The surface elements becomes more and more relevant in small bodies:

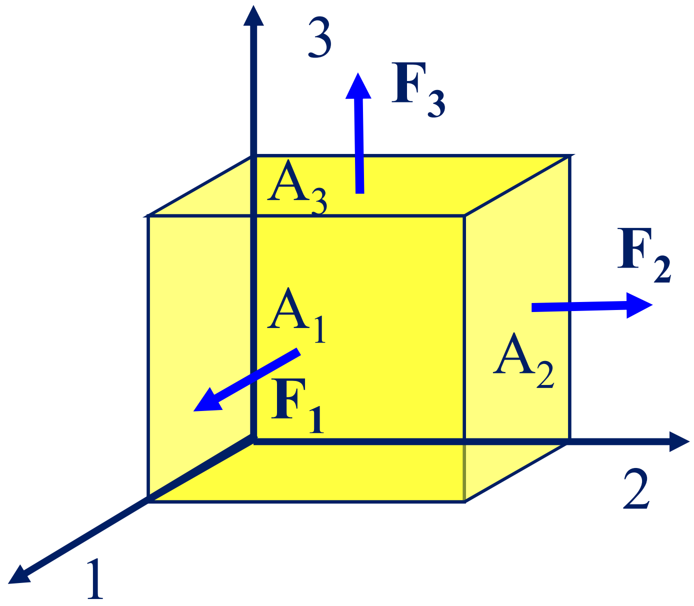
  l = 1 m → Surface/Volume = 6 m^{-1};

  l = 1 cm → Surface/Volume = 6 cm^{-1} = 600 m^{-1}

- Forces applied to the body (e.g, gravity)
- Forces applied at the surfaces (e.g., pressure, bending, twisting)



- Normal stresses (or *axial*)

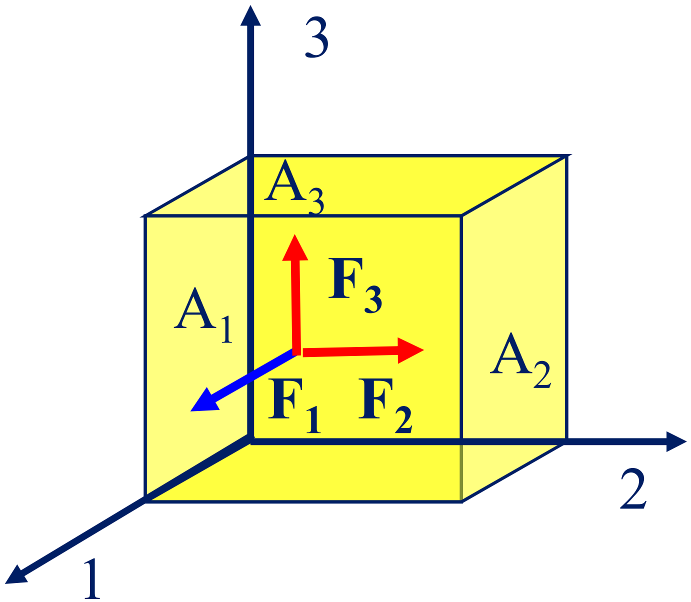


$$\sigma_{11} = F_1/A_1$$

$$\sigma_{22} = F_2/A_2$$

$$\sigma_{33} = F_3/A_3$$

- Shear stresses



σ_{31}

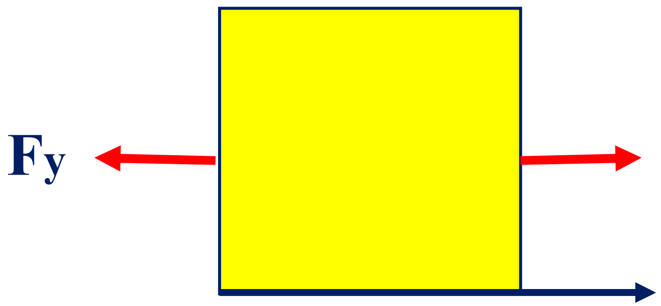
σ_{21}

σ_{ij}

Equilibrium condition: in order to have no accelerations of the body, all forces and moments must balance:

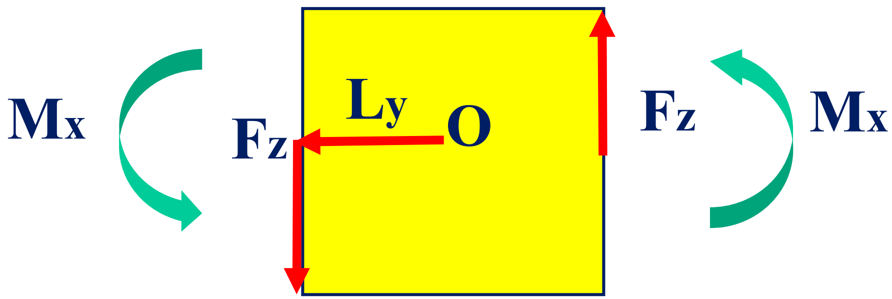
i) The surface axial forces need to be equal on two opposite planes:

$$\Sigma F_x = 0$$
$$\Sigma F_y = 0$$
$$\Sigma F_z = 0$$



ii) The shear forces, even if balanced, would induce a rotation moment:

$$M_x = 2 * L_y F_z$$



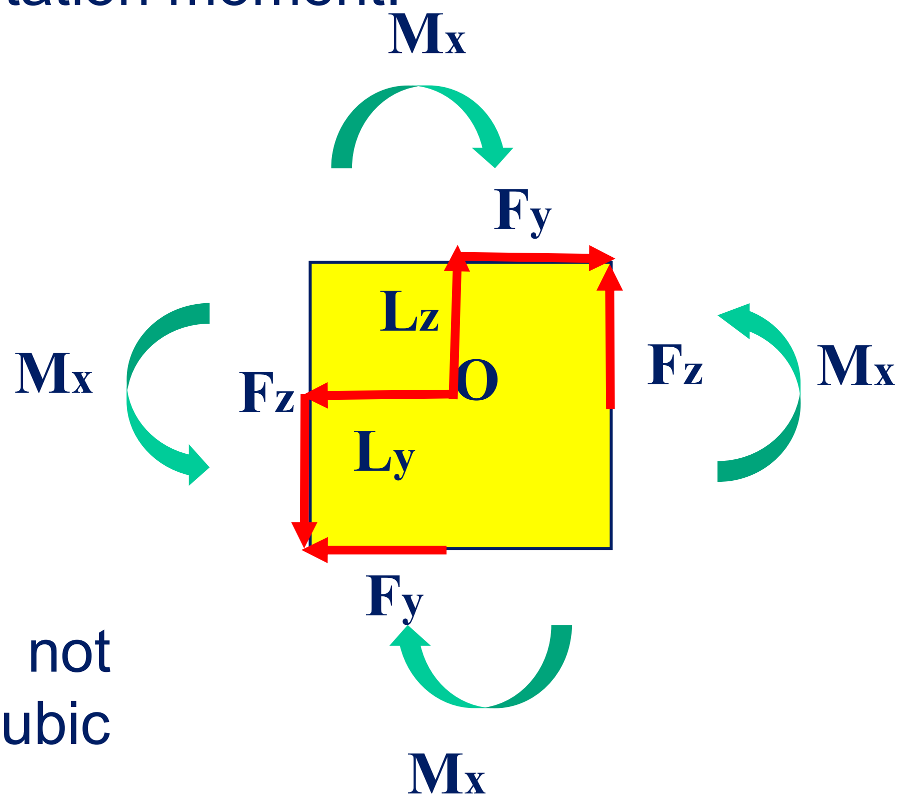
Equilibrium condition:

In order to have no accelerations of the body one must consider the action of a second couple of shear forces on the dual planes, balancing the rotation moment:

$$\Sigma M_x = 2 * L_y F_z - 2 * L_z F_y = 0$$

$$\Rightarrow \quad \sigma_{ij} = \sigma_{ji}$$

(for the above to apply it is not necessary to consider a cubic block)

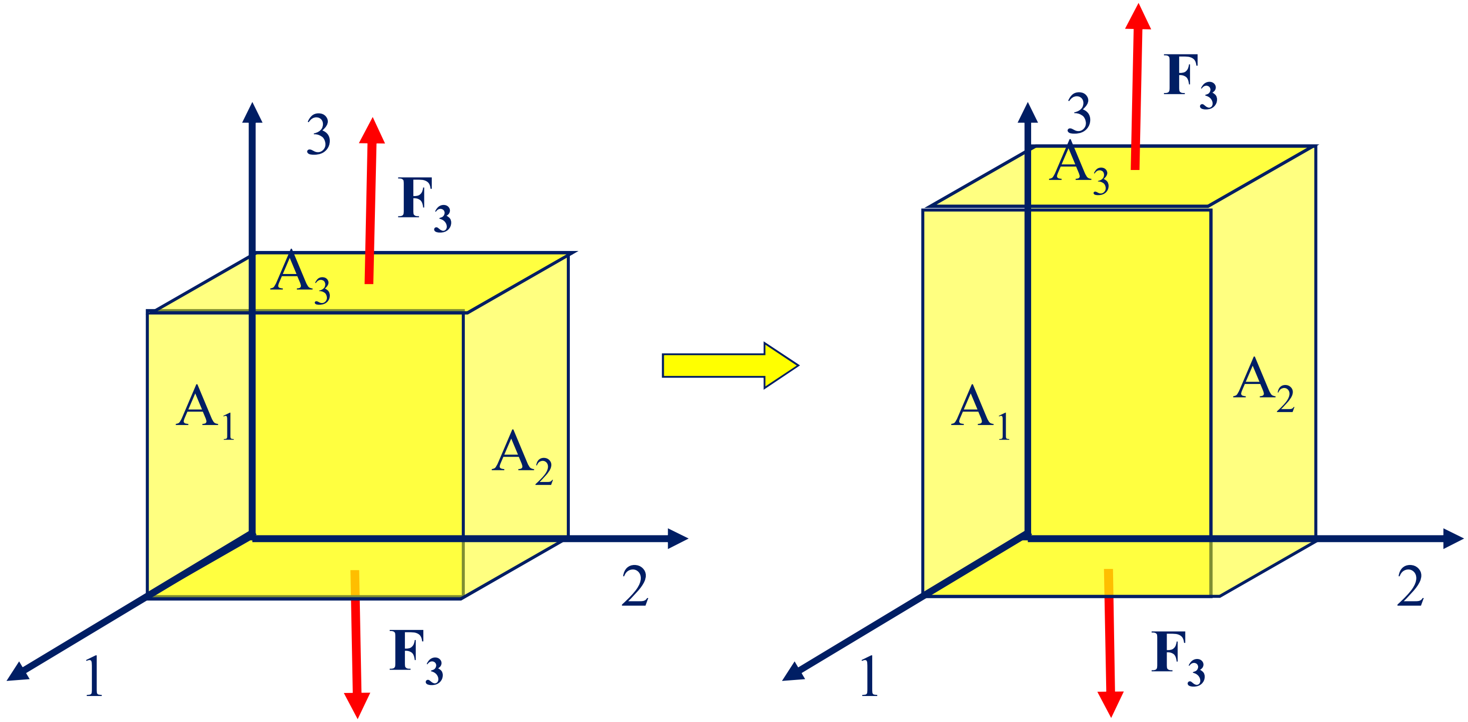


STRESS TENSOR

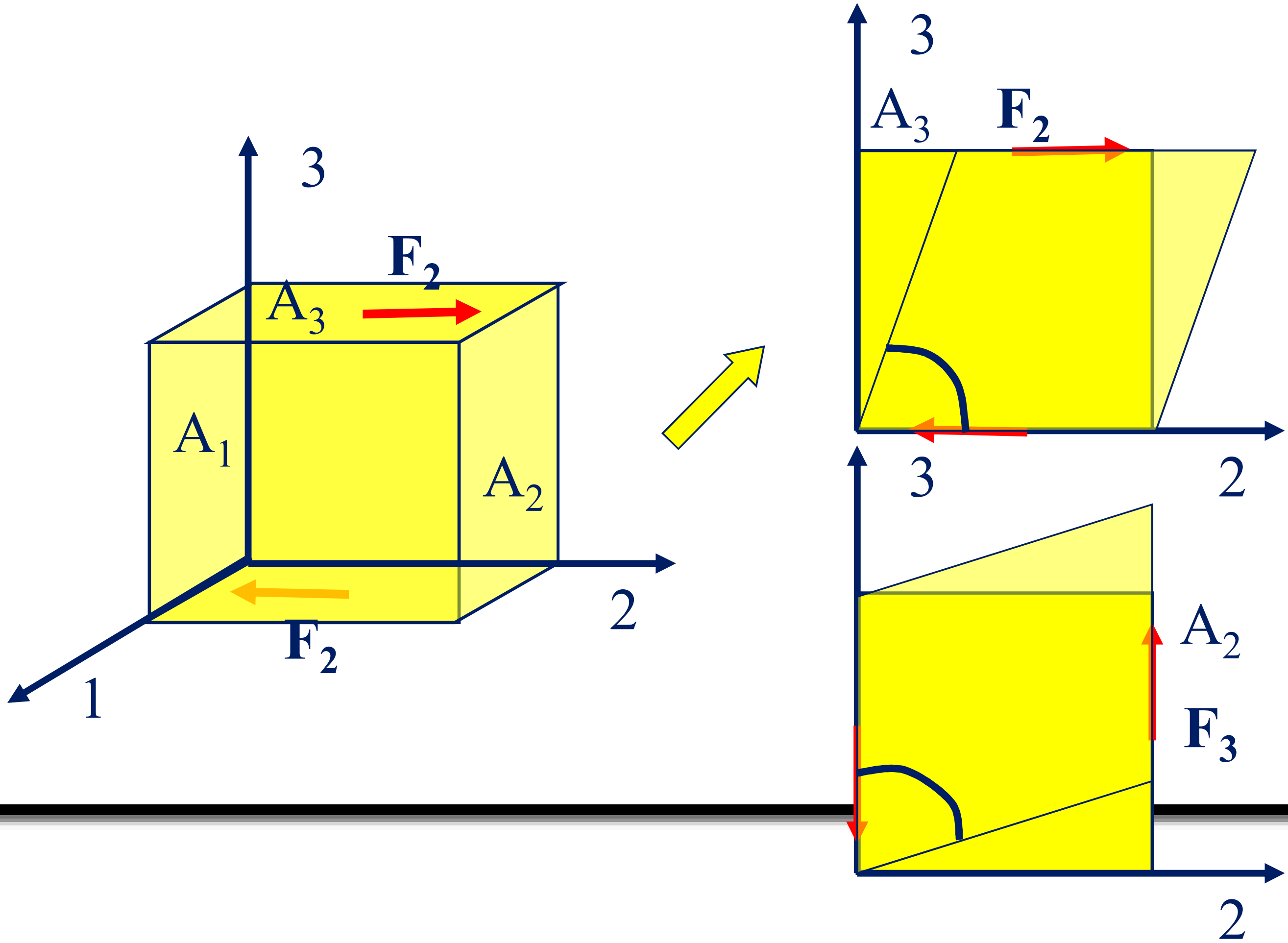
$$\begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33}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

$$\begin{pmatrix} 1 & 6 & 5 \\ & 2 & 4 \\ & & 3 \end{pmatrix} \Rightarrow \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{pmatrix}$$

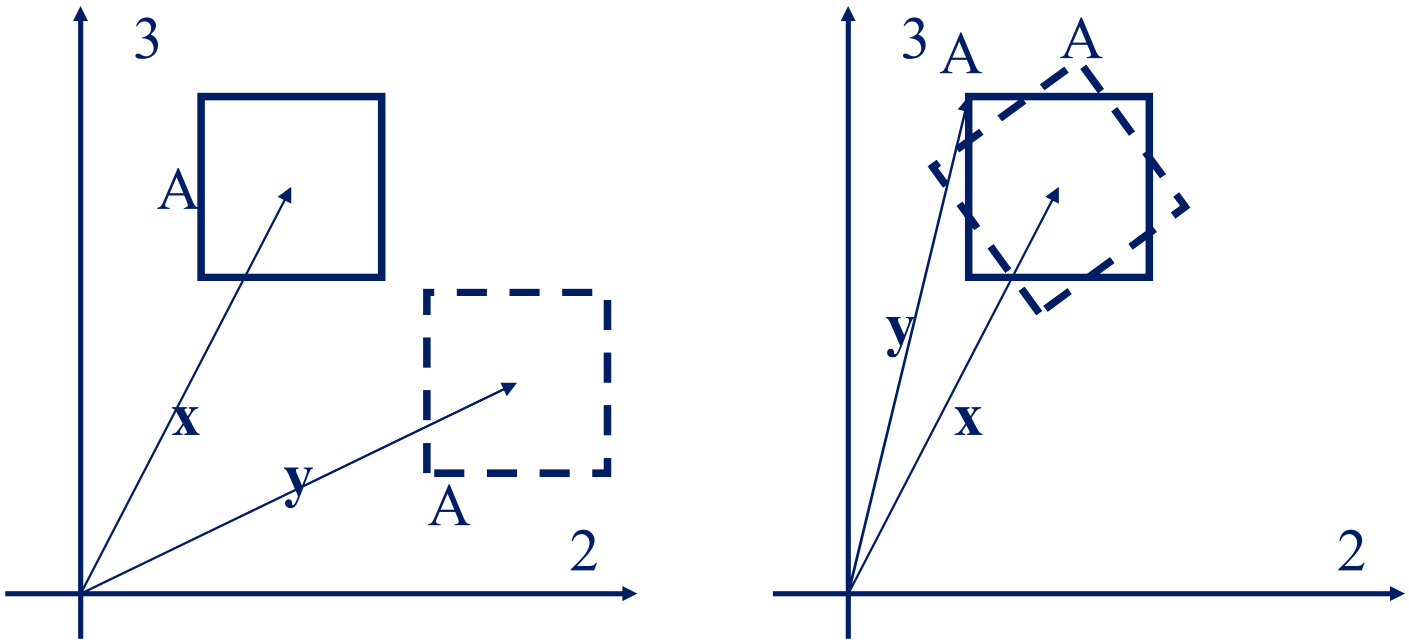
- Deformations due to axial stresses



- Deformations due to shear stresses



Strain tensor



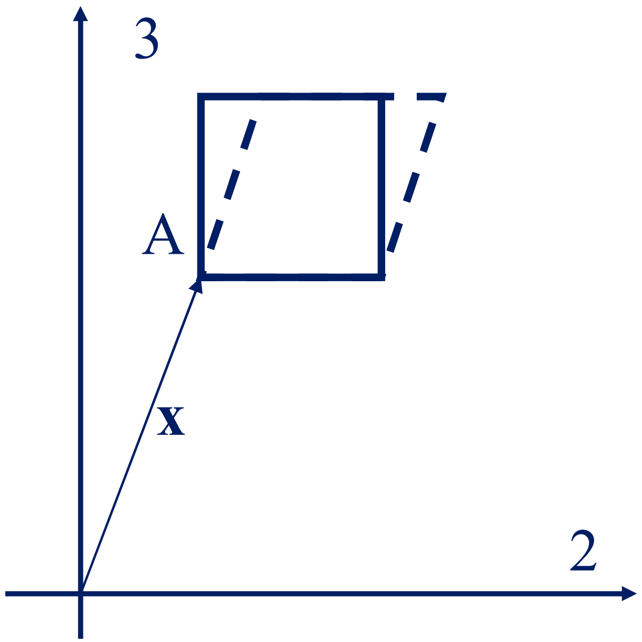
$$\boldsymbol{t} = (\boldsymbol{y} - \boldsymbol{x}) \qquad \boldsymbol{r} = \boldsymbol{\omega} \wedge (\boldsymbol{y} - \boldsymbol{x})$$

Traslation and Rotation without deformation

$$\overline{\overline{\omega}} = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix}$$

$$\boldsymbol{u} = \boldsymbol{dx} + \overline{\overline{\omega}}\boldsymbol{dx}$$

Deformation → Strain tensor



$$\boldsymbol{u} = \boldsymbol{u}_0 + \left(\nabla_{\boldsymbol{x}}\boldsymbol{u}\right)d\boldsymbol{x}$$

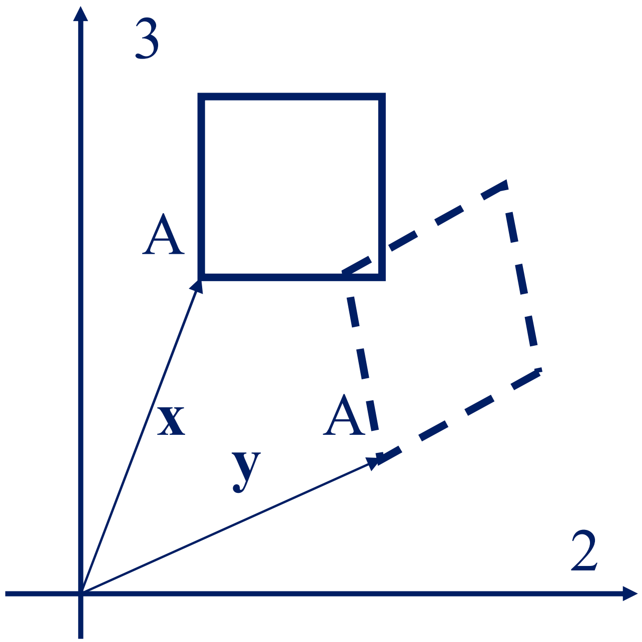
$$\left(\nabla_{\boldsymbol{x}}\boldsymbol{u}\right)_{ij} = \frac{\partial u_i}{\partial x_j} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right)$$

$$\left(\nabla_{\boldsymbol{x}}\boldsymbol{u}\right)_{ij} = \frac{\partial u_i}{\partial x_j} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right)$$

$$\left(\nabla_{\boldsymbol{x}}\boldsymbol{u}\right)_{ij} = \varepsilon_{ij} + \omega_{ij}$$

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \Rightarrow \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \varepsilon_{23} \\ \varepsilon_{13} \\ \varepsilon_{12} \end{pmatrix}$$

Traslation, Rotation and Deformation



$$\boldsymbol{u} = \boldsymbol{u}_0 + \overline{\overline{\boldsymbol{\omega}}}\boldsymbol{dx} + \overline{\overline{\boldsymbol{\varepsilon}}}\boldsymbol{dx}$$

Generalized Hooke's Law
(compliance matrix for isotropic materials)

$$\varepsilon_{hk} = \sum_{ij} b_{hk,ij}\sigma_{ij}$$

$$\begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \varepsilon_{23} \\ \varepsilon_{13} \\ \varepsilon_{12} \end{pmatrix} = \begin{pmatrix} b_{11} & b_{12} & b_{12} & 0 & 0 & 0 \\ b_{12} & b_{11} & b_{12} & 0 & 0 & 0 \\ b_{12} & b_{12} & b_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & b_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & b_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & b_{44} \end{pmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{pmatrix}$$

Generalized Hooke's Law

- The inverse of the compliance matrix is called *stiffness matrix.*
- Elastic constants in isotropic materials:

$$b_{11} = 1 / E , \qquad b_{12} = - \nu / E , \qquad b_{44} = 1 / G$$

  - E = Young's modulus
  - ν = Poisson's coefficient
  - G = shear modulus

The equations of linear elasticity

$$F_i^b = \int_V f_i^b dV$$

$$F_i^s = \int_S \sigma_{ij} n_j dS = \int_V \sum_{j=1}^{3} \frac{\partial \sigma_{ij}}{\partial x_j} dV$$

$$\sum_{j=1}^{3} \frac{\partial \sigma_{ij}}{\partial x_j} + f_i^b = \rho \dot{v}_i$$

Mechanical Sensors

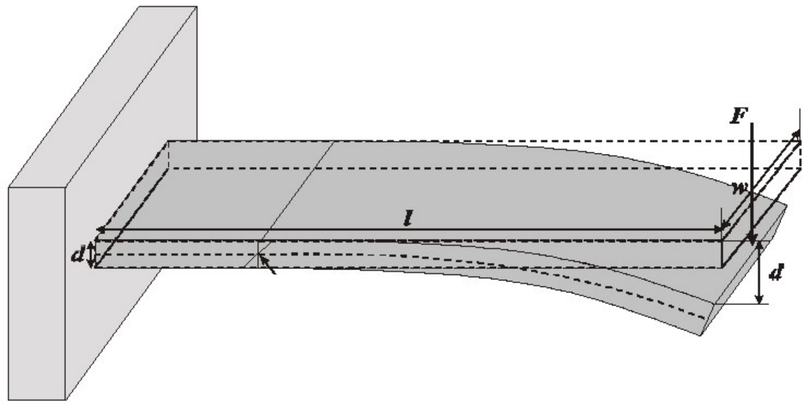
Characterization of mechanical sensors

- the measurand and the physical structures

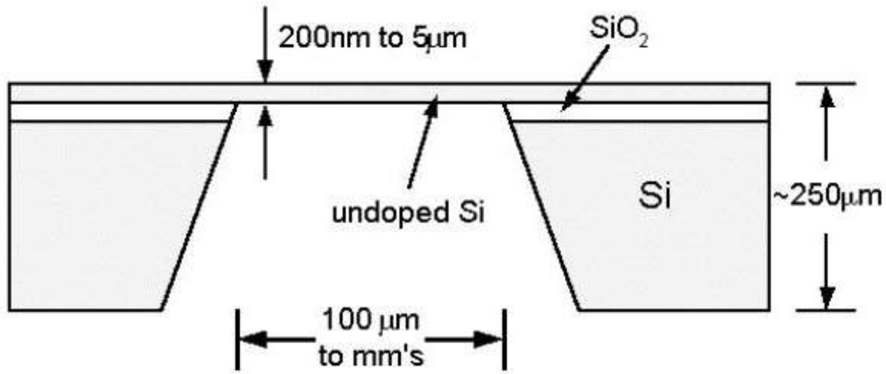
1. Most relevant mechanical signals, their units in the S.I., and ranges for specific applications
2. Definition of the stress and strain tensors
3. Description of the structural elements mainly used in solid-state sensors (beams & plates)

Mechanical structures used in MEMS sensors

Cantilever beams



Membranes/Plates



Cantilever beam (fixed end beam)

Type of loads

a. concentrated load (single force)

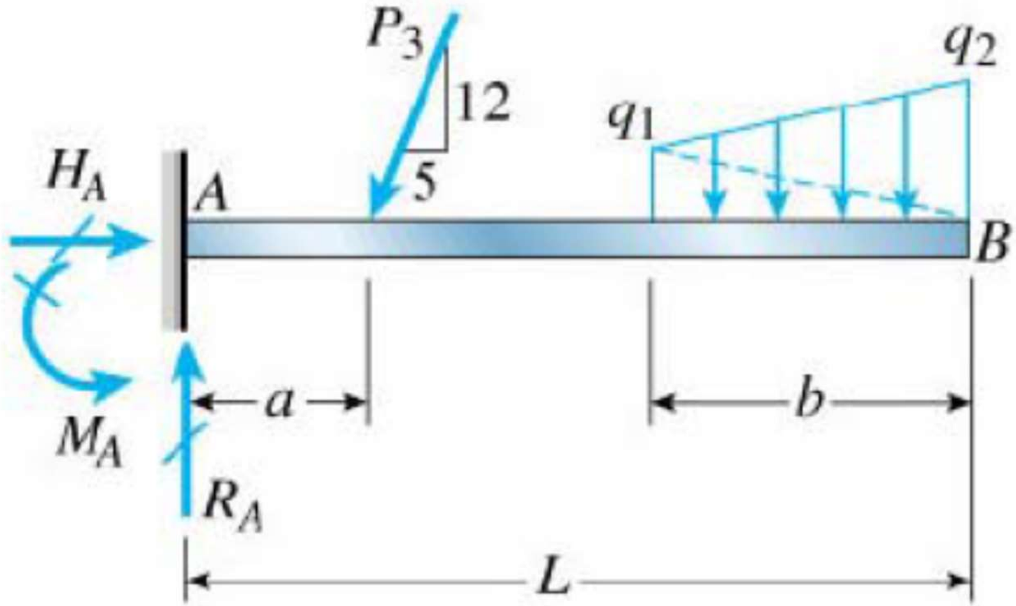
b. distributed load (measured by their intensity) :

uniformly distributed load (uniform load)

linearly varying load

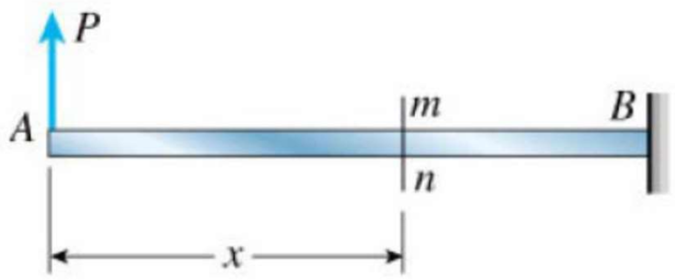
Reactions:

The fixed end prevents translations and rotations

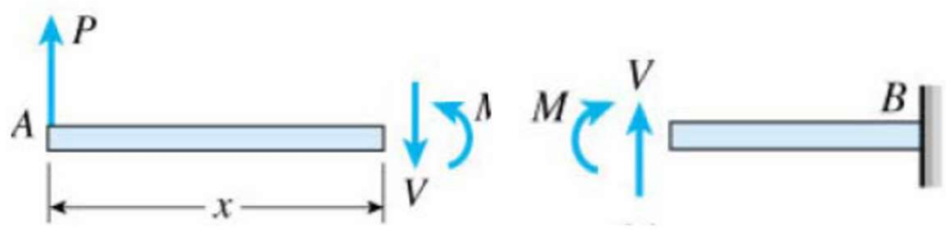


Cantilever beam (fixed end beam)

Shear Forces and Bending Moments



concentrated load P applied at the end



$$\Sigma F_y = 0 \qquad V = P$$

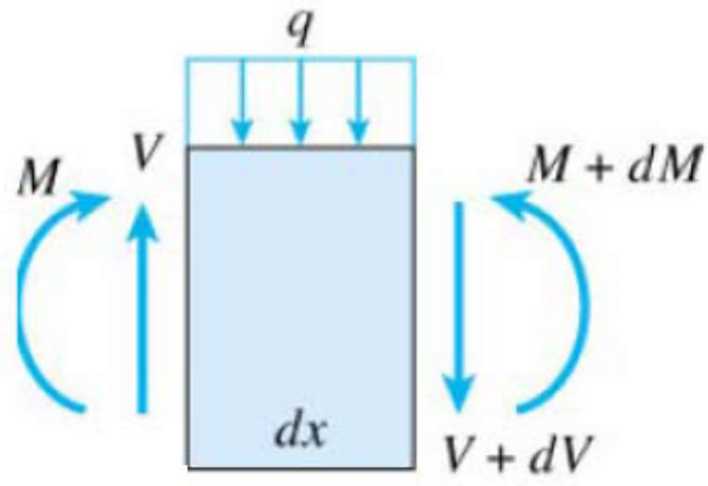
$$\Sigma M = 0 \qquad M = P\,x$$

Cantilever beam (fixed end beam)

Relationships Between Loads, Shear Forces, and Bending Moments

consider an element of a beam of length dx

subjected to distributed loads q



$$\Sigma F_y = 0 \qquad V - q\,dx - (V + dV) = 0$$

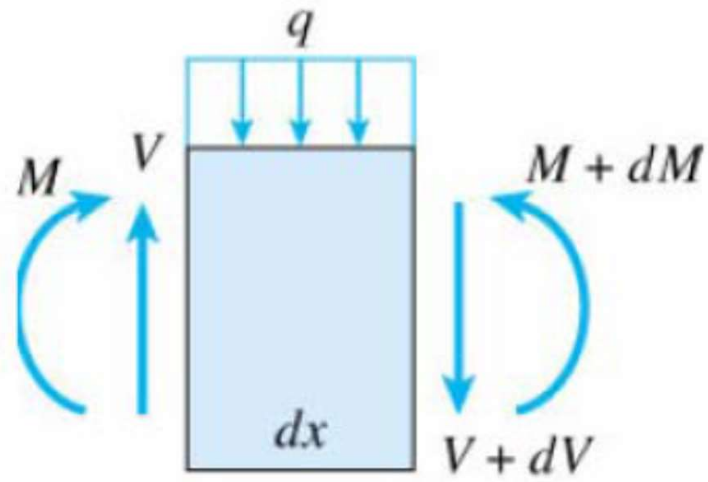
or $\qquad \boldsymbol{dV / dx = -q}$

Cantilever beam (fixed end beam)

Relationships Between Loads, Shear Forces, and Bending Moments

consider an element of a beam of length dx

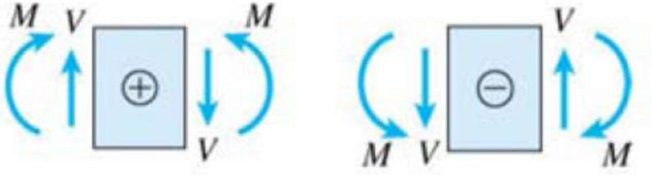
subjected to distributed loads q



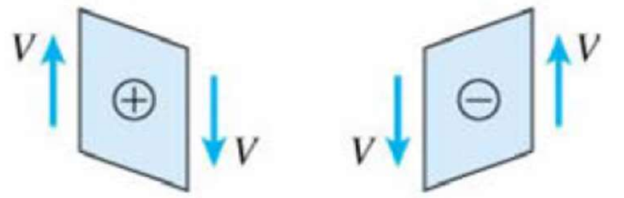
$\Sigma M = 0$ $\quad - M - q\,dx\,(dx/2) - (V + dV)\,dx + M + dM = 0$

or $\quad \boldsymbol{dM / dx = V}$

Cantilever beam (fixed end beam)
Deformations

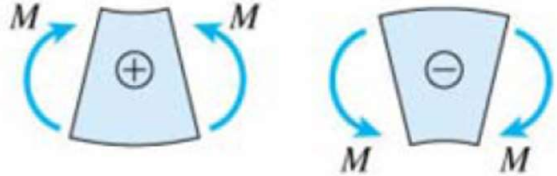


the shear force tends to rotate the material clockwise is defined as positive



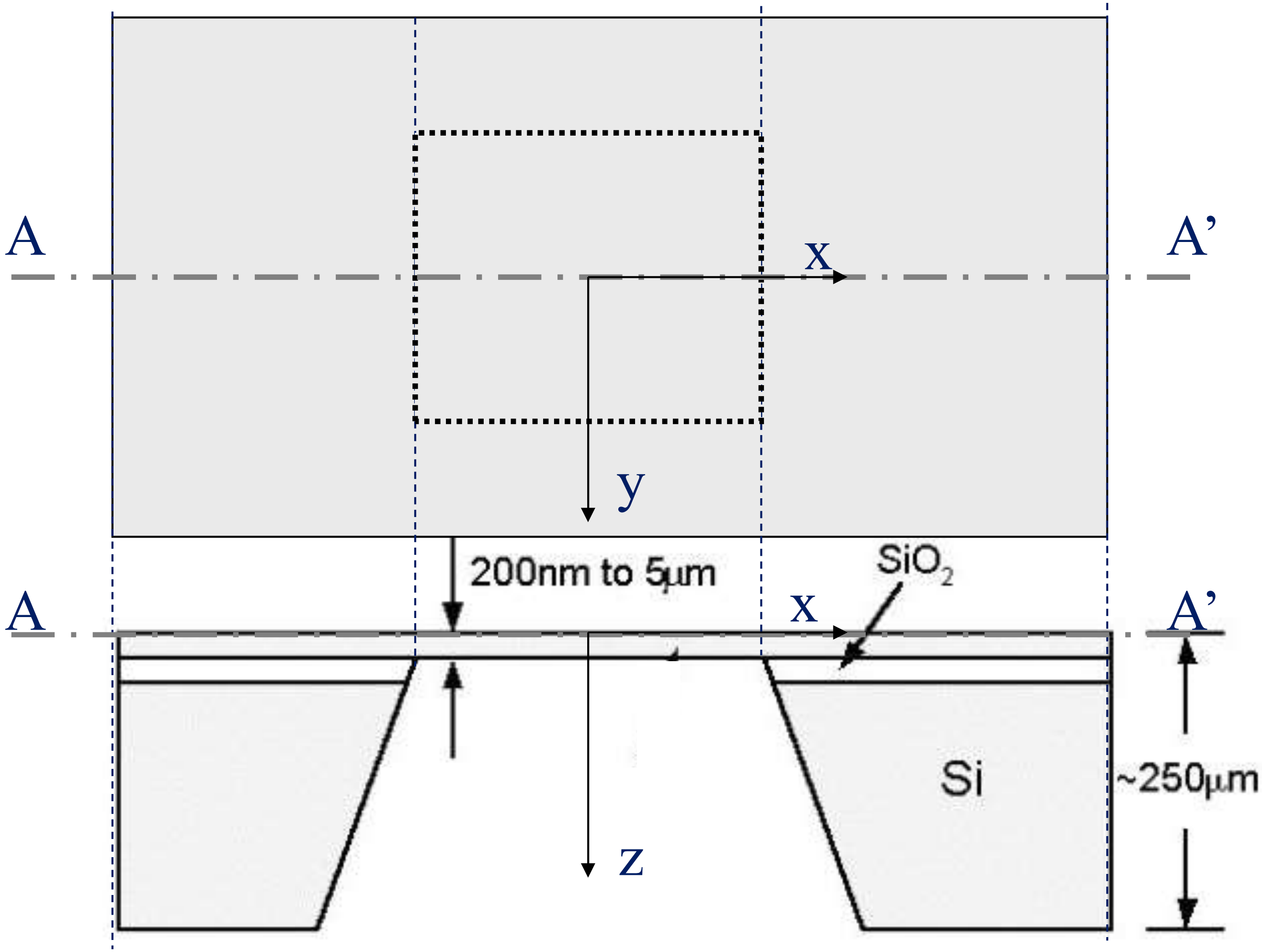
(a)

the bending moment tends to compress the upper part of the beam and elongate the lower part is defined as positive



(b)

MEMS plates in silicon



Plates (basic concepts of plate bending)

A plate can be considered the two-dimensional extension of a beam in simple bending.

Both plates and beams support loads transverse or perpendicular to their plane and through bending action.

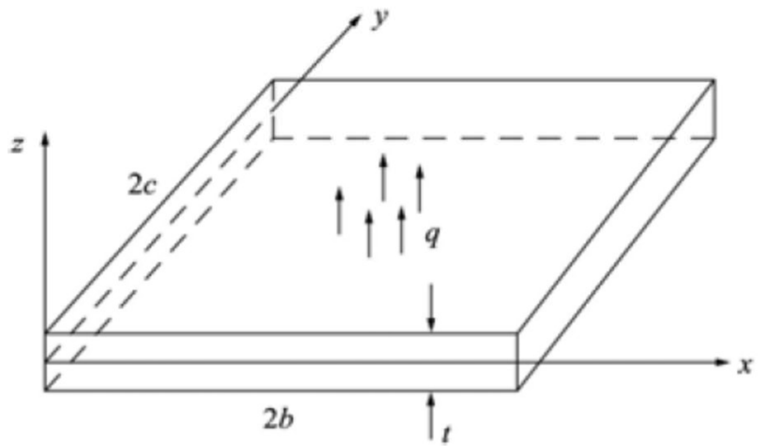
A plate is a flat (if it were curved, it would be a shell).

A beam has a single bending moment resistance, while a plate resists bending about two axes and has a twisting moment.

We will consider the classical thin-plate theory or Kirchhoff plate theory.

Plates (basic concepts of plate bending)

Consider the thin plate in the *x-y* plane of thickness *t* measured in the *z* direction shown in the figure below:



The plate surfaces are at $z = \pm t/2$, and its midsurface is at $z = 0$.

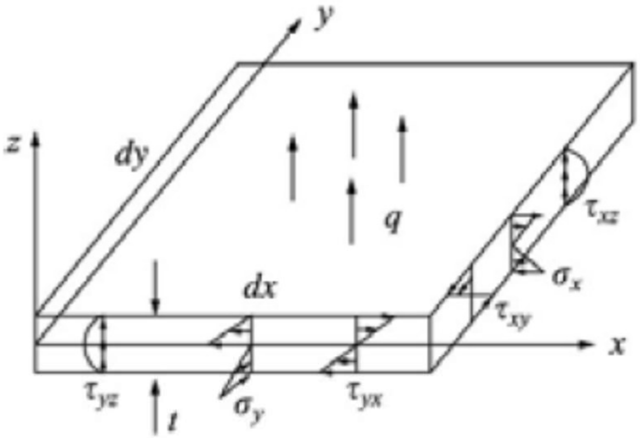
1. The plate thickness is much smaller than its inplane **dimensions** *b* and *c* (that is, $t \ll b$ or c

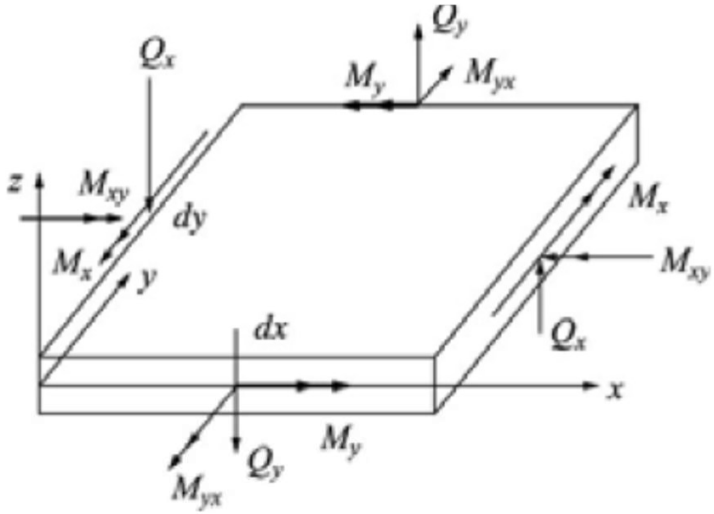
Plates (basic concepts of plate bending)

Kirchhoff Assumptions

1. Normals remain normal. This implies that transverse shears strains $\gamma_{yz} = 0$ and $\gamma_{xz} = 0$. However γ_{xy} does not equal to 0
2. Thickness changes can be neglected and normals undergo no extension. This means that $\varepsilon_z = 0$.
3. Normal stress σ_z has no effect on in-plane strains ε_x and ε_y in the stress-strain equations and is considered negligible.
4. Therefore, the in-plane deflections in the x and y directions at the midsurface, $t = 0$, are assumed to be zero; $u(x, y, 0) = 0$ and $v(x, y, 0) = 0$.

Plates (basic concepts of plate bending)





The governing differential equations are:

$$\frac{\partial Q_x}{\partial x} + \frac{\partial Q_y}{\partial y} + q = 0$$

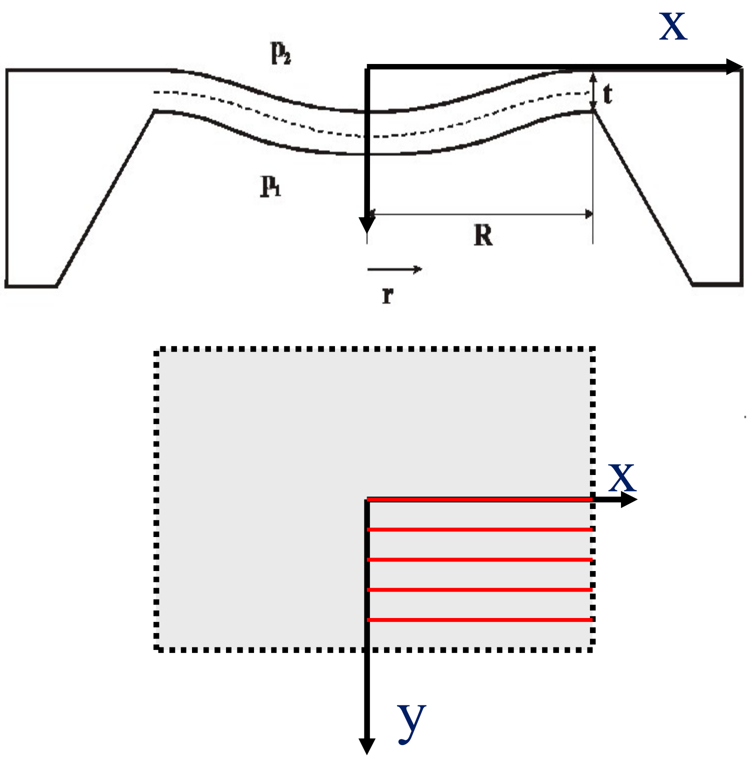
$$\frac{\partial M_x}{\partial x} + \frac{\partial M_{xy}}{\partial y} - Q_x = 0$$

$$\frac{\partial M_y}{\partial y} + \frac{\partial M_{xy}}{\partial x} - Q_y = 0$$

where q is the transverse distributed loading and Q_x and Q_y are the transverse shear line loads.

Solution of the plate bending problem

(S.K.Clark &K.D. Wise, IEEE Tr. ED 26, 1979)



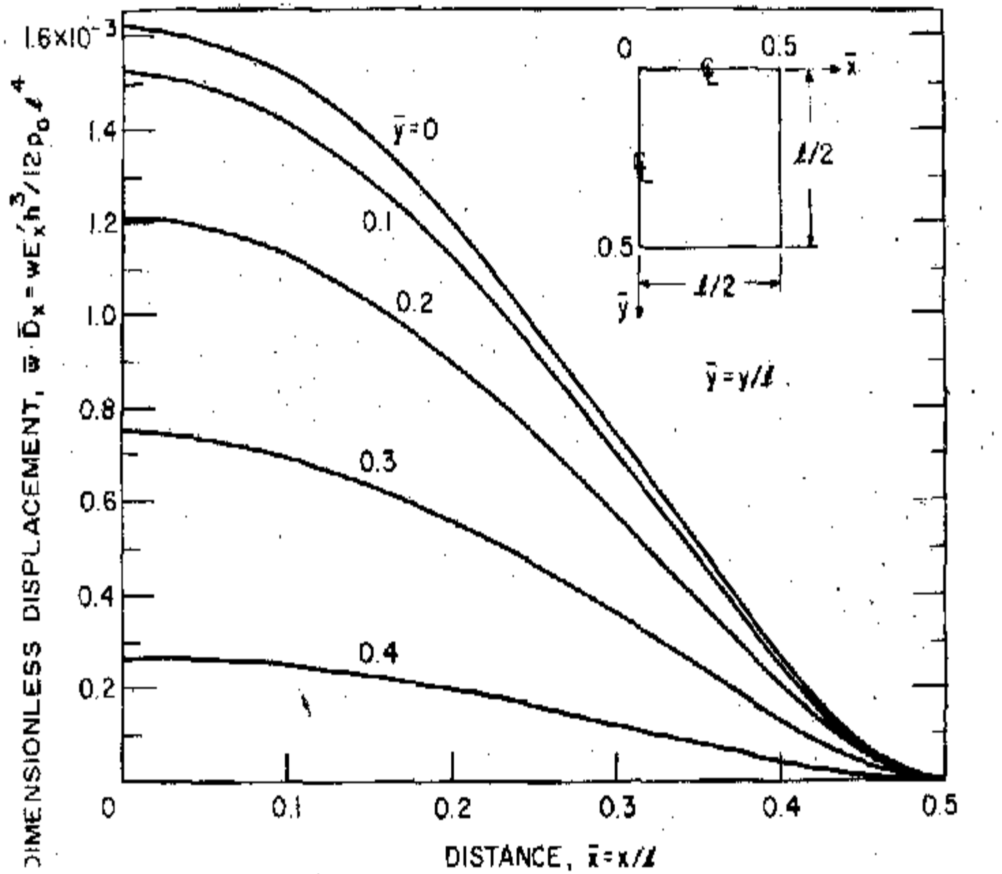
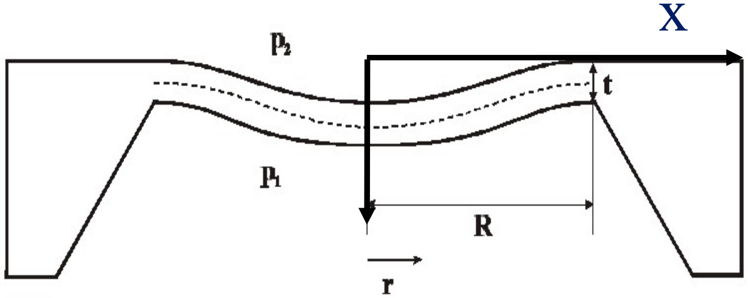
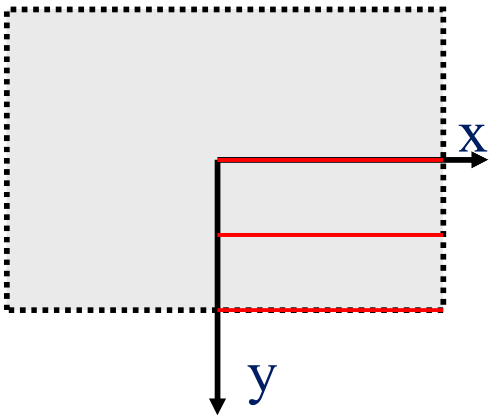


Fig. 4. Dimensionless displacement of a square silicon diaphragm having built-in edges as a function of position on the diaphragm.

Solution of the plate bending problem

(S.K.Clark &K.D. Wise, IEEE Tr. ED 26, 1979)





$$\sigma_{xxmax} = 0.3\ p\ (L/H)^2$$

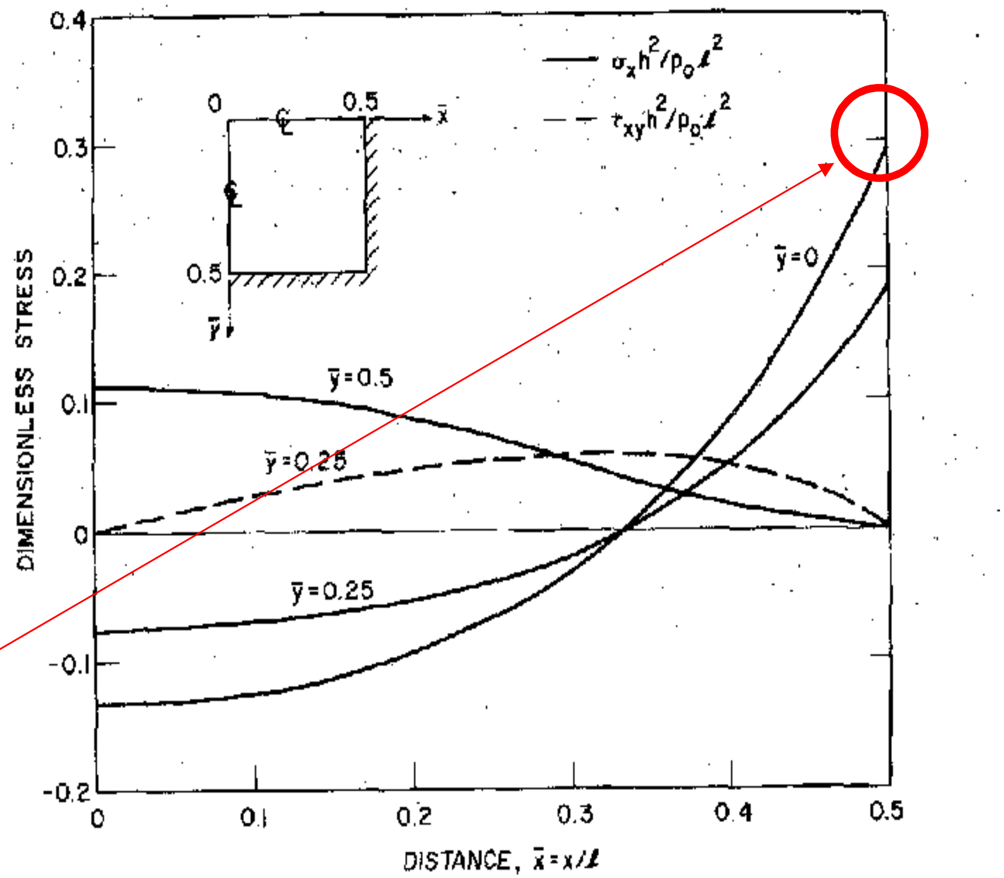
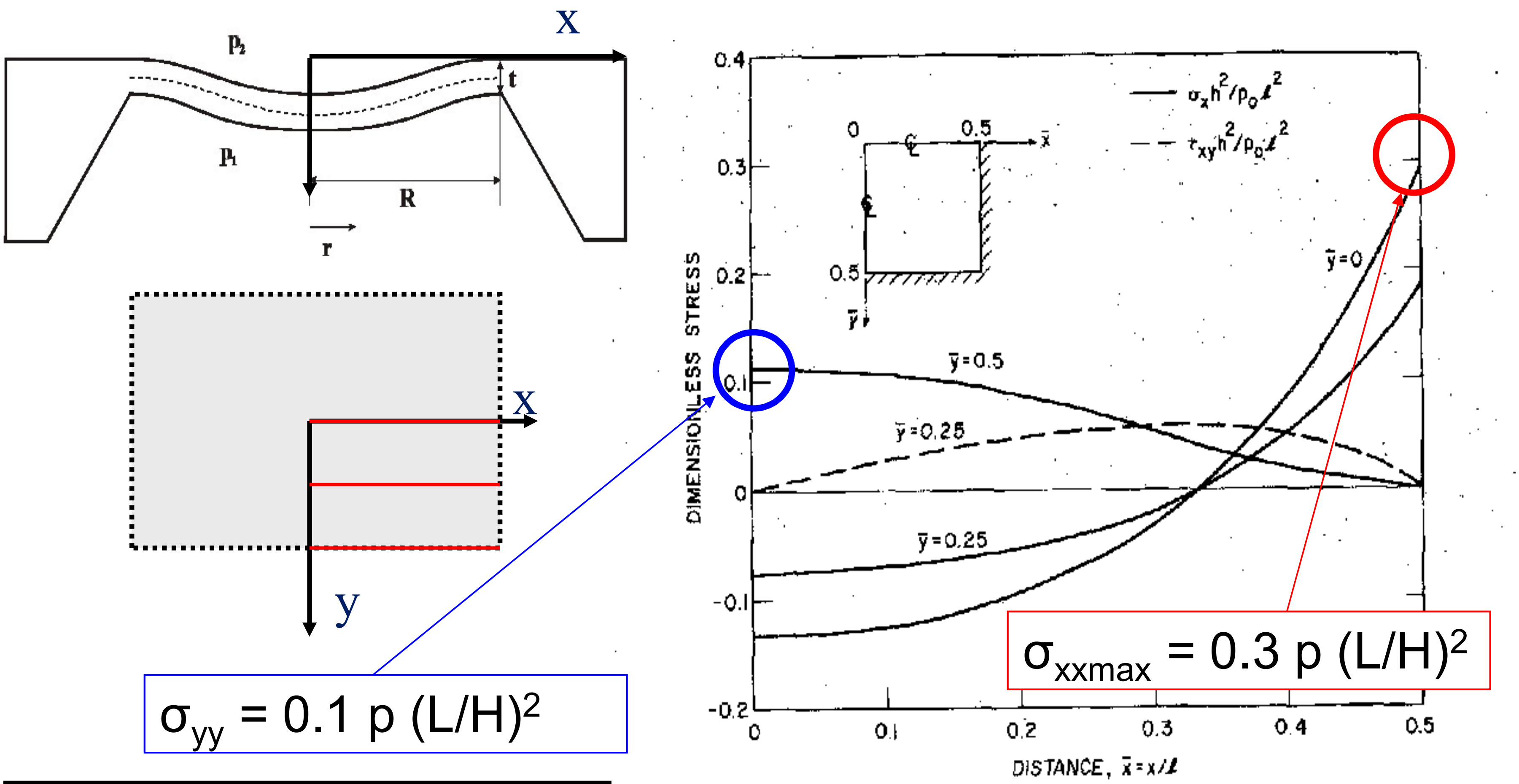


Fig. 5. Dimensionless stress distributions on a silicon diaphragm having built-in edges.

Solution of the plate bending problem

(S.K.Clark &K.D. Wise, IEEE Tr. ED 26, 1979)



$\sigma_{xxmax} = 0.3\ p\ (L/H)^2$

$\sigma_{yy} = 0.1\ p\ (L/H)^2$

Fig. 5. Dimensionless stress distributions on a silicon diaphragm having built-in edges.