Cristals, tensors, elasticity & piezoelectricity

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1 Description of cristals

1.1 Properties

The attenuation of elastic waves is smallest for the most ordered states of matter:

- In air (in a gas), the practical limit is a few 100 kHz;
- In water (in liquids), the practical limit is a few 100 MHz;
- With solid-state crystals, the practical limit is a few 10 GHz, at least. The piezoelectric effect can be used to generate and detect elastic waves at those frequencies.

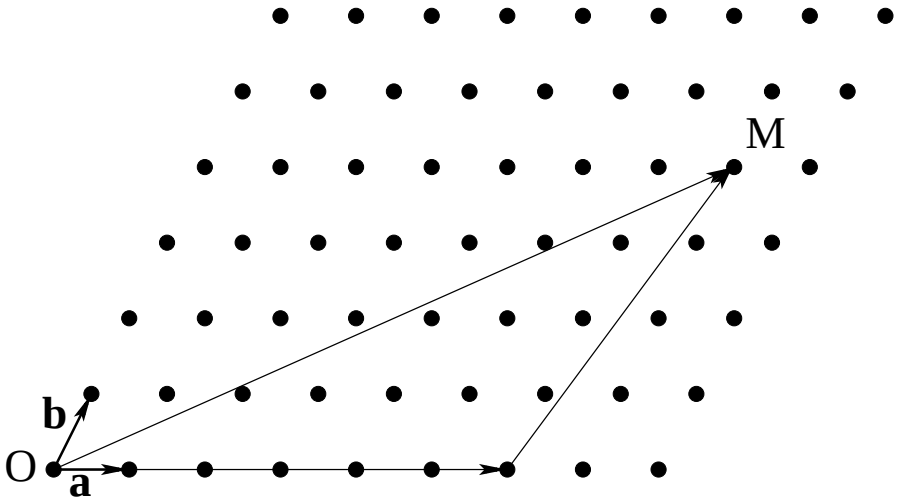
The symmetry of crystals directly dictates the anisotropic properties of elastic waves. Crystals can be classified according to their orientation symmetry. The microscopic symmetry reflects in the macroscopic physical properties.

A crystal is homogeneous: the behaviors of different samples with the same orientation and obtained from the same crystal are identical.

The concept of tensor is the natural mathematical language to describe physical properties and their relations with symmetry.

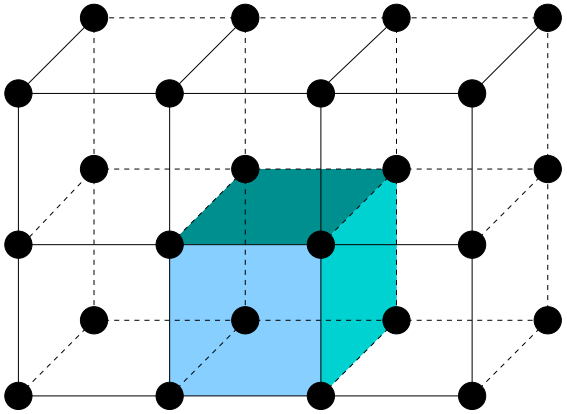
1.2 Crystal array (lattice)

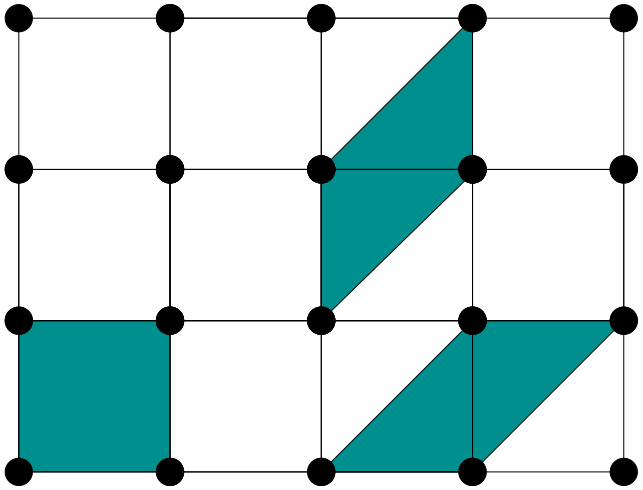
There exist an infinity of nodes, or points that are images in an elementary translation:
$\overrightarrow{\mathrm{OM}} = m\boldsymbol{a} + n\boldsymbol{b} + p\boldsymbol{c}$ with m, n, p indices
All nodes have the same atomic environment.



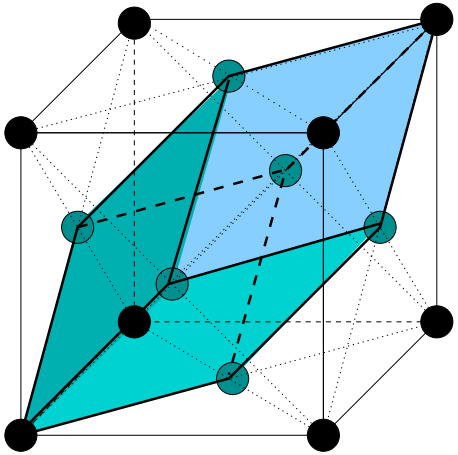
1.3 Unit cell

The periodic array (=lattice) can be seen as a stack of unit cells, parallelograms whose vertices are nodes.
A unit cell built from 3 basis vectors is primitive (it contains a single node).





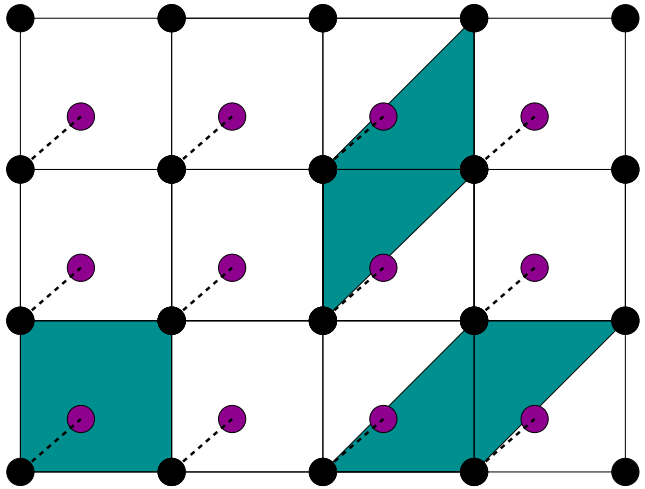
Face centered cubic lattice:
an additional node appears at the centre of each face of the cube.
The cubic unit cell is 4 times too wide.
The primitive unit cell is a rhomboedron (a polyhedron whose faces are rhombuses).

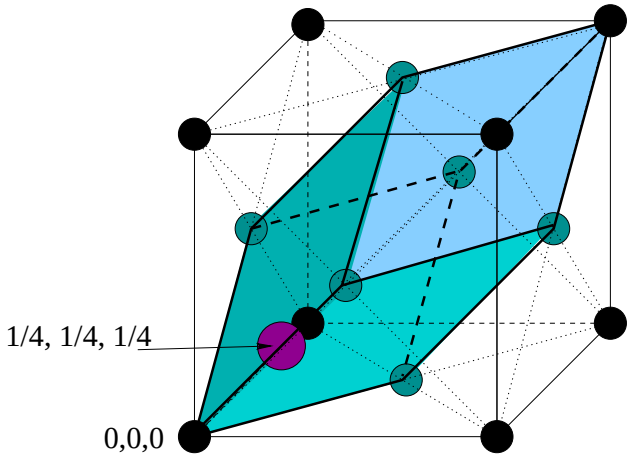


1.4 Basis

A basis is a set of atoms positioned at the nodes of the lattice.

- The basis can be composed of a single atom
  - → face centered cubic (fcc): Cu, Ag, Al, Ni, Pt...
  - → centered cubic (cc): Li, Na, K, Cr...
- The basis can be composed of a repetition of the same atom
  - → diamond: fcc lattice + 1 atom at 1/4,1/4,1/4 (Si, Ge...)
- The basis can be composed of different atoms (ZnS, AsGa)





2 Orientation symmetry

2.1 The 14 Bravais lattices

- The 14 Bravais lattices are the only possible manners to distribute in 3D spaces an infinite array of nodes having the same environment.

- There are conventionally 7 lattice systems.

- They are further separated into possibly 3 lattice centerings:

  → centered (I)

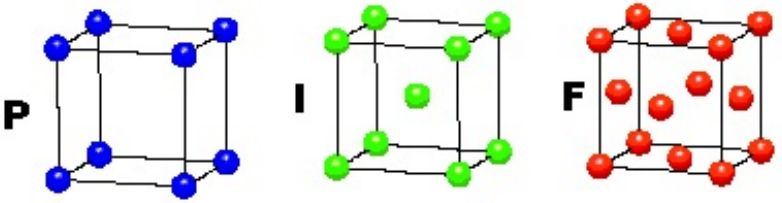
  → one node on two opposite faces (C)

  → face centered (F)

CUBIC

$a = b = c$

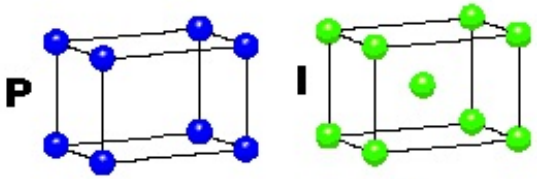
$\alpha = \beta = \gamma = 90°$



TETRAGONAL

$a = b \neq c$

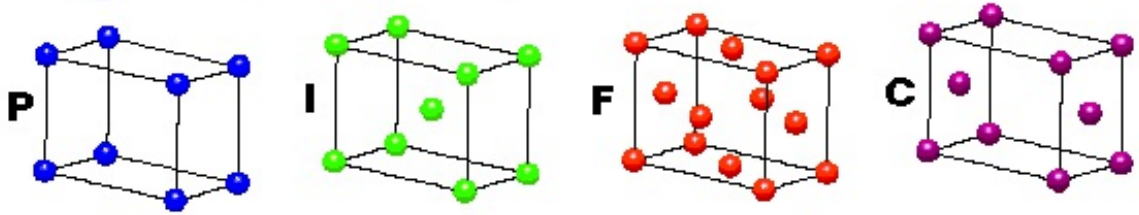
$\alpha = \beta = \gamma = 90°$



ORTHORHOMBIC

$a \neq b \neq c$

$\alpha = \beta = \gamma = 90°$

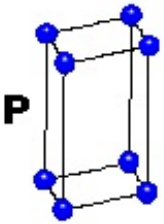


HEXAGONAL

$a = b \neq c$

$\alpha = \beta = 90°$

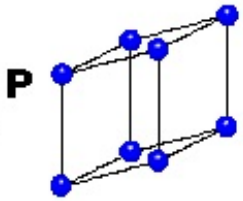
$\gamma = 120°$



TRIGONAL

$a = b = c$

$\alpha = \beta = \gamma \neq 90°$

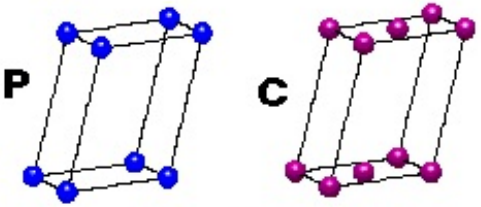


MONOCLINIC

$a \neq b \neq c$

$\alpha = \gamma = 90°$

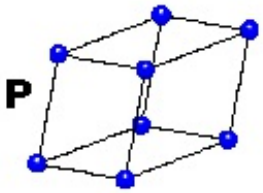
$\beta \neq 120°$



TRICLINIC

$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma \neq 90°$



4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices

2.2 The 32 point groups (point symmetry classes)

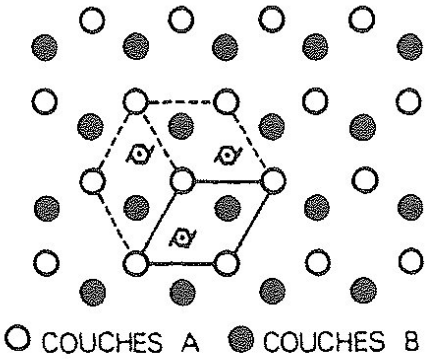
- Adjoining the basis at each node, the overall symmetry of the crystal is possibily reduced.

- A crystal is not necessarily centro-symmetric (piezoelectric crystals, for instance).

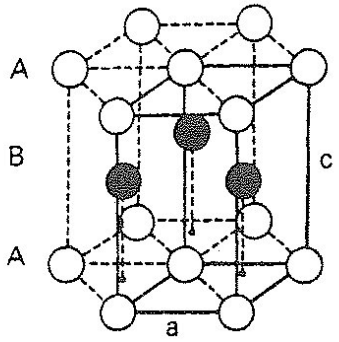
- The 32 point groups of crystals imply the anisotropy of the material constants, and hence the anisotropy of propagation velocity (see Section 5).

3 Examples of structures

3.1 Compact hexagonal structure

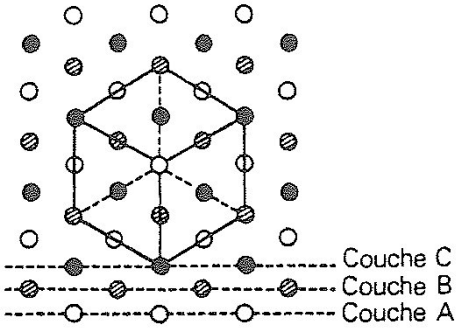


a

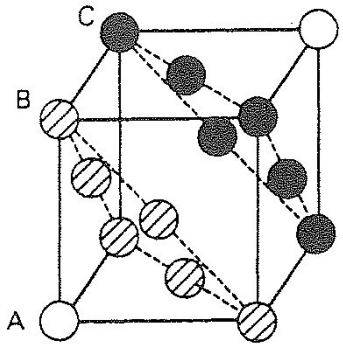


b

3.2 Face centered cubic (fcc)

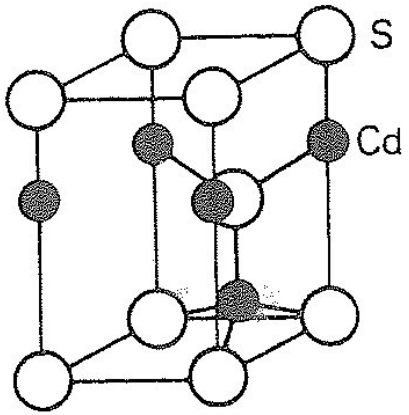


a

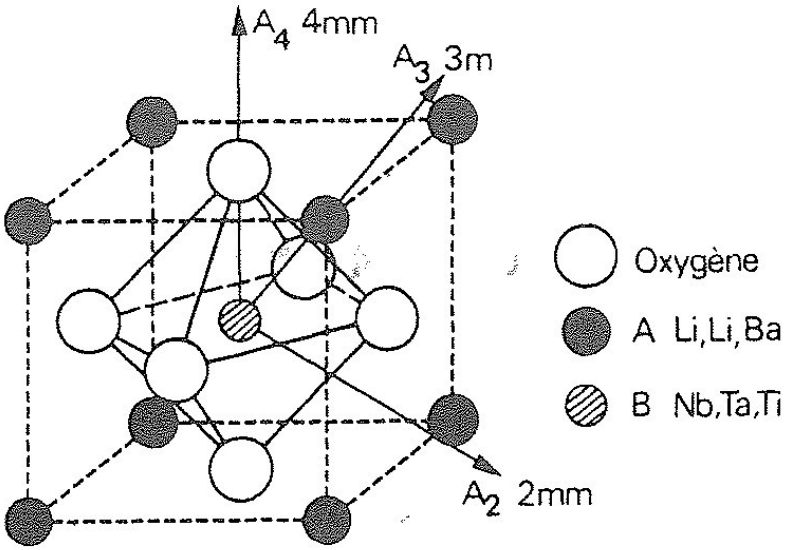


b

3.3 ZnO, AlN, CdS: hexagonal system, 6mm symmetry



3.4 $LiNbO_3$ and $LiTaO_3$: trigonal system, 3m symmetry



4 Introduction to tensors

4.1 Linear relations in anisotropic media

Inside a crystal, a cause applied in a given direction generally induces an effect oriented in another direction. For instance, the relation between electrical polarization and electric field is

$$\boldsymbol{D}=\varepsilon\,\boldsymbol{E} \text{ ou } \begin{pmatrix} D_1 \\ D_2 \\ D_3 \end{pmatrix}=\begin{pmatrix} \varepsilon_{11}\,\varepsilon_{12}\,\varepsilon_{13} \\ \varepsilon_{21}\,\varepsilon_{22}\,\varepsilon_{23} \\ \varepsilon_{31}\,\varepsilon_{32}\,\varepsilon_{33} \end{pmatrix}\begin{pmatrix} E_1 \\ E_2 \\ E_3 \end{pmatrix} \text{ or } D_i=\varepsilon_{ij}\,E_j \tag{1}$$

The first two notations make use of vectors and matrices. The last one is tensorial and uses the implied summation convention on repeated indices (or Einstein convention).

D_i and E_j are order 1 tensors; ε_{ij} is an order 2 tensor. The order is the number of indices.

Giving the components of a tensor is not sufficient in order to determine it. It is furthermore necessary to specify how the tensor transforms in a given transformation of the reference frame: the physical significance does not change when axes are rotated, only the representation of the tensor is changed!

4.2 Reference frame transform matrix

Let $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$ and $\boldsymbol{e}'_1, \boldsymbol{e}'_2, \boldsymbol{e}'_3$ be two reference frames. The components of the new reference frame in the old reference frame form a matrix α such that (a matrix, not a tensor!)

$$\boldsymbol{e}'_i = \alpha_i^k \, \boldsymbol{e}_k \text{ with } \alpha = \begin{pmatrix} \alpha_1^1 & \alpha_1^2 & \alpha_1^3 \\ \alpha_2^1 & \alpha_2^2 & \alpha_2^3 \\ \alpha_3^1 & \alpha_3^2 & \alpha_3^3 \end{pmatrix} \tag{2}$$

Reciprocally $\boldsymbol{e}_k = \beta_k^j \, \boldsymbol{e}'_j$ with $\alpha_i^k \, \beta_k^j = \delta_{ij}$ and δ_{ij} the Kronecker symbol. If the reference frames are orthonormal then $\beta = \alpha^T$ (T: transposition operator).

The coordinates of a vector obey the transformation law:

$$x'_i = \beta_k^i \, x_k \text{ with } \boldsymbol{x} = x_k \, \boldsymbol{e}_k = x'_i \, \boldsymbol{e}'_i \tag{3}$$

In case the reference frames are orthonormal, then the coordinates of a vector obey the same transformation law as the basis vectors: $x'_i = \alpha_i^k \, x_k$.

4.3 Definition of a tensor

- Any scalar physical quantity (temperature, energy, etc.) is invariant of the chosen reference frame: $f(x_1,x_2,x_3)=f(x'_1,x'_2,x'_3)$; it is an order 0 tensor.
- An order 1 tensor (i.e. a vector) transforms in a reference frame change as the basis vectors, or

$$A'_i=\alpha_i^k\,A_k \tag{4}$$

- An order 2 tensor is a set of 9 components A_{ij} that transforms according to

$$A'_{ij}=\alpha_i^k\,\alpha_j^l\,A_{kl} \tag{5}$$

- The definition extends smoothly to an arbitrary order, for instance at order 3:

$$A'_{ijk}=\alpha_i^l\,\alpha_j^p\,\alpha_k^q\,A_{lpq} \tag{6}$$

- The gradient of a vector, $\partial A_i/\partial x_k$, is an order 2 tensor.
- The trace A_{ii} of an order 2 tensor, A_{ij}, is an order 0 tensor (a scalar).
- The linear relation between two tensors is also a tensor. For instance $D_i=\varepsilon_{ij}\,E_j$ implies that ε_{ij} is an order 2 tensor.

5 Elasticity

5.1 Deformations

Consider a point $\boldsymbol{x}$ with coordinates x_1, x_2, x_3. Displacements $\boldsymbol{u}$ are a function of $\boldsymbol{x}$, hence $u_i(x_j + \mathrm{d}x_j) = u_i(x_j) + \frac{\partial u_i}{\partial x_j}\,\mathrm{d}x_j$ to first order. $\frac{\partial u_i}{\partial x_j}$, the displacement gradient, is an order 2 tensor.

This gradient is separated into a symmetric part (the strain tensor S_{ij}) and an antisymmetric part

$$\frac{\partial u_i}{\partial x_j} = S_{ij} + \Omega_{ij} \text{ with } S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \text{ and } \Omega_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right) \tag{7}$$

Only the symmetric part of the displacement gradient actually measures of local volume change of the lattice. The antisymmetric part measures local rotations.

The dilation (i.e. the local variation of the volume) is $S_{ii} = S_{11} + S_{22} + S_{33} = \nabla.\boldsymbol{u}$, that is the trace of the displacement tensor.

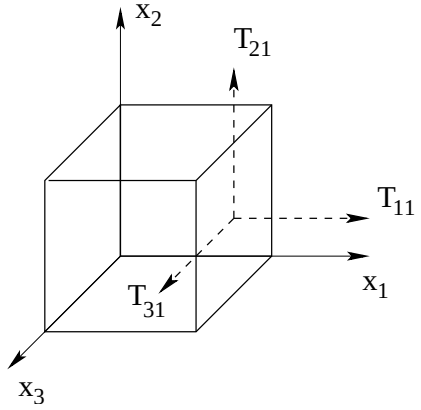
For elastic waves, the diagonal components S_{11}, S_{22}, S_{33} are linked to longitudinal motion, whereas the non-diagonal components $S_{ij}, i \neq j$ are linked to shear motion.

5.2 Stress

Contrary to fluids, shear forces in solids are transmitted through a surface. Three independent forces apply to a surface: a traction-compression force and 2 shear forces.

On the face orthogonal to axis x_1 of an elementary cube, the force per unit surface (i.e. the mechanical traction) is $T_{11} + T_{21} + T_{31}$ (with similar formulas for faces orthogonal to axes x_2 and x_3).

T_{ij} is a symmetrical order 2 tensor, the stress tensor. For an arbitrary elementary surface with normal $\boldsymbol{l}$, the mechanical traction is $T_{ik}\, l_k$.



The elastodynamic equation is (with f_i some body forces)

$$\frac{\partial T_{ik}}{\partial x_k} + f_i = \rho \frac{\partial^2 u_i}{\partial t^2} \tag{8}$$

5.3 Hooke's law

Experiment indicates that the elastic behavior of most solids in the limit of small deformations follows Hooke's law :

$$T_{ij} = c_{ijkl}\, S_{kl} \tag{9}$$

This amounts to stating that stress is a linear function of strain.

c_{ijkl} is the elastic tensor, of order 4. It has *a priori* $3^4 = 81$ components. The symmetry of both T_{ij} et S_{kl}, however, implies

$$c_{jikl} = c_{ijkl} \text{ and } c_{ijlk} = c_{ijkl} \tag{10}$$

There are thus 36 independent components at most. Moreover, it can be shown that the elastic tensor is symmetric, $c_{\mathrm{ijkl}}{=}c_{\mathrm{klij}}$, hence 21 independent components remain.

As a whole, the actual number of independent components (or independent constants) is a function of the symmetry of the crystal.

5.4 Contracted notation (or matrix notation)

Thanks to the symmetry relations we note

$$(11) \longleftrightarrow 1 \; ; \; (22) \longleftrightarrow 2 \; ; \; (33) \longleftrightarrow 3$$
$$(23)=(32) \longleftrightarrow 4 \; ; \; (31)=(13) \longleftrightarrow 5 \; ; \; (12)=(21) \longleftrightarrow 6 \qquad (11)$$

$$T_{ij} = T_I \; ; \; c_{ijkl} = c_{IJ} \; ; \; T_I = c_{IJ} S_J$$
$$S_1 = S_{11} \; ; S_2 = S_{22} \; ; S_3 = S_{33} \; ; S_4 = 2S_{23} \; ; S_5 = 2S_{31} \; ; S_6 = 2S_{12} \qquad (12)$$

Material	Class	Elastic constants (10^{10} N/m^2)						ρ (10^3 kg/m^3)
cubic ou isotropic		c_{11}	c_{12}	c_{44}				
AsGa	$\bar{4}\,3m$	11.88	5.38	2.83				5.307
SiO_2	isotrope	7.85	1.61	3.12				2.203
Si	$m3m$	16.56	6.39	7.95				2.329
hexagonal		c_{11}	c_{12}	c_{13}	c_{33}	c_{44}		
PZT-4	trans. iso.	13.9	7.8	7.4	11.5	2.6		7.5
ZnO	$6mm$	21.0	12.1	10.5	21.1	4.2		5.676
trigonal		c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{14}	
Al_2O_3	$\bar{3}\,m$	49.7	16.3	11.1	49.8	14.7	-2.3	3.986
$LiNbO_3$	$3m$	20.3	5.3	7.5	24.5	6.0	0.9	4.7
quartz α (SiO_2)	32	8.7	0.7	1.2	10.7	5.8	-1.8	2.648

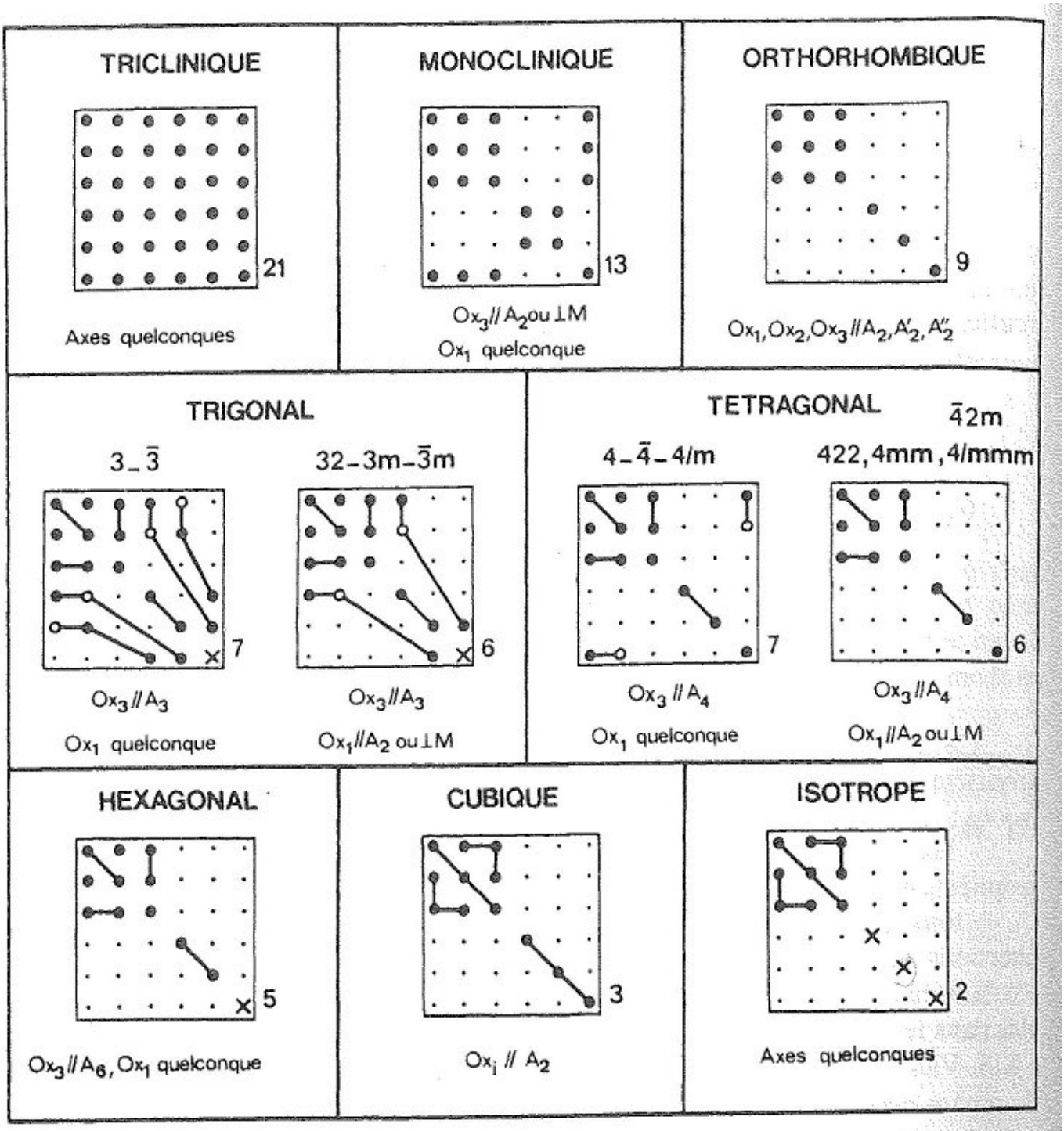


FIG. 3. 9. *Composantes $c_{\alpha\beta}$ du tenseurs des rigidités élastiques suivant les systèmes de symétrie avec les axes de référence de la figure 2. 22.*

composante – *non nulle* : ● ○ – *nulle* : •

composantes – *égales* : ●—● – *opposées* : ●—○

– *égales à* $(c_{11} - c_{12})/2$: ×

La symétrie par rapport à la diagonale principale n'est pas mentionnée. Le nombre de composantes indépendantes est indiqué, en bas, à droite de chaque ensemble.

6 Piezoelectricity

6.1 Physical origin of piezoelectricity

Direct piezoelectric effect: if a stress or strain is applied, an electrical polarization appears (i.e., a non symmetrical deformation of the atomic unit cell and/or of the distribution of bound electrons).
Inverse piezoelectric effect (or Lippman effect): An applied electric field induces a stress or strain.
The piezoelectric effect is only observed in non centrosymmetric crystals.

6.2 Constitutive relations

Considering the linear regime only, and choosing strain and electric field as the state variables,

$$T_{ij} = c_{ijkl}\, S_{kl} - e_{kij}\, E_k \tag{13}$$
$$D_i = e_{ikl}\, S_{kl} + \varepsilon_{ij}\, E_j \tag{14}$$

or in contracted notation for the mechanical part

$$T_I = c_{IJ}\, S_J - e_{kI}\, E_k \tag{15}$$
$$D_i = e_{iJ}\, S_J + \varepsilon_{ij}\, E_j \tag{16}$$

Piezoelectric tensor $e_{ikl} = e_{iJ}$ is symmetrical vs. the last 2 indices only.

6.3 Quasi-static approximation

As a consequence of piezoelectric coupling, an electromagnetic wave travels along with the elastic wave. Maxwell's equations in a dielectric (or insulator) are :

$$\nabla\times\boldsymbol{E}=-\frac{\partial\boldsymbol{B}}{\partial t}\;;\nabla\times\boldsymbol{H}=\frac{\partial\boldsymbol{D}}{\partial t}\;;\nabla.\boldsymbol{D}=0\;;\nabla.\boldsymbol{H}=0\;;\boldsymbol{B}=\mu_0\,\boldsymbol{H} \tag{17}$$

The involved frequencies are quite small compared to optical waves, resulting in negligible temporal derivatives:

$$\nabla\times\boldsymbol{E}=-\mathrm{i}\omega\boldsymbol{B}\simeq 0 \text{ and } \nabla\times\boldsymbol{H}=\mathrm{i}\omega\boldsymbol{D}\simeq 0$$

This approximation decouples electric and magnetic fields. In addition, as the electric field is irrotational there exists a scalar potential ϕ such that $\boldsymbol{E}=-\nabla\phi$. The constitutive relations become

$$T_I = c_{IJ}\,S_J+e_{kI}\,\phi_{,k} \tag{18}$$
$$D_i = e_{iJ}\,S_J-\varepsilon_{ij}\,\phi_{,j} \tag{19}$$

6.4 Matrix representation of constitutive relations

Grouping tensors in equations (15-16) into a table of constants:

c_{11} c_{12} . . . . c_{12} c_{22} . . . . c_{16} . . . . c_{66}	e_{11} e_{21} e_{31} e_{12} . . . . e_{16} . e_{36}
e_{11} e_{12} . . . e_{16} e_{21} . . . . . e_{31} . . . . e_{36}	ε_{11} ε_{12} ε_{13} ε_{12} . . ε_{13} . ε_{33}

This representation is quite handy to identify possible couplings given the crystal symmetry, but also in order to represent « material constants » data in a numerical simulation program.

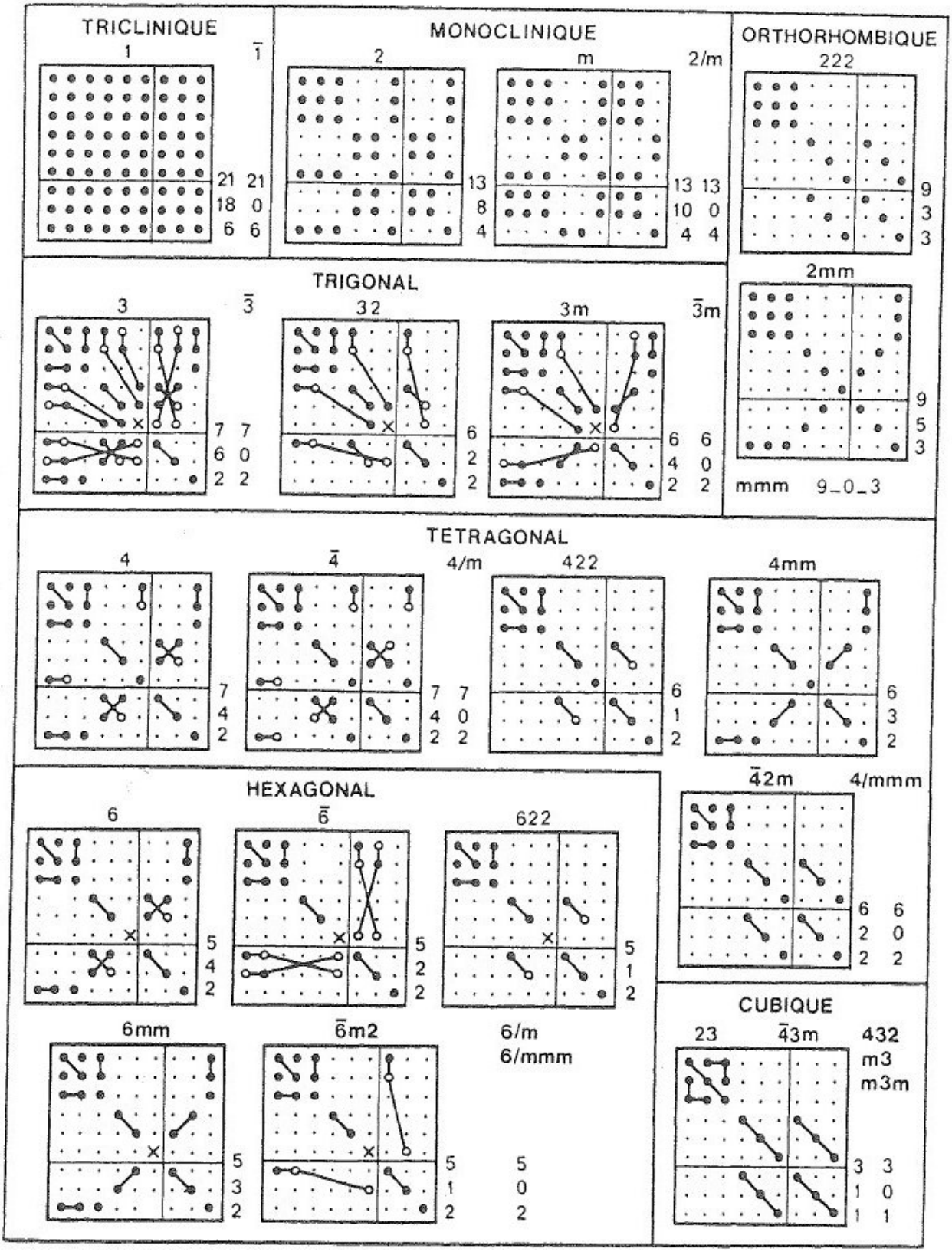


FIG. 3. 14. *Composantes des tenseurs élastiques, piézoélectriques, diélectriques suivant les classes de symétrie avec les axes de référence de la figure 2. 22.*

composante – non nulle : ● ○ *– nulle :* ·

composantes – égales : ●—● *– opposées :* ●—○ *– égales à* $(c_{11} - c_{22})/2$ *:* ×

La symétrie par rapport à la diagonale principale n'est pas mentionnée. Les nombres de constantes élastiques, piézoélectriques et diélectriques indépendantes sont indiqués à droite de chaque ensemble.

MATÉRIAUX	CLASSE	CONSTANTES PIÉZOÉLECTRIQUES (C/m^2)						PERMITTIVITÉS ($10^{-11}F/m$)	
Système cubique		e_{14}						ε^S	
Arséniure de gallium (AsGa)	$\bar{4}3m$	− 0,16						9,73	
Oxyde de bismuth et de germanium ($Bi_{12}GeO_{20}$)	23	0,99						34,2	
Système hexagonal		e_{15}		e_{31}		e_{33}		ε^S_{11}	ε^S_{33}
Céramique PZT-4	trans. isotrope	12,7		− 5,2		15,1		650	560
Oxyde de zinc (ZnO)	6*mm*	− 0,59		− 0,61		1,14		7,38	7,83
Sulfure de cadmium (CdS)	6*mm*	− 0,21		− 0,24		0,44		7,99	8,44
Système tétragonal		e_{14}	e_{15}	e_{31}	e_{33}			ε^S_{11}	ε^S_{33}
Paratellurite (TeO_2)	422	0,22	0	0	0			20	22
Titanate de baryum ($BaTiO_3$)	4*mm*	0	21,3	− 2,65	3,64			1 744	97
Système trigonal		e_{11}	e_{14}	e_{15}	e_{22}	e_{31}	e_{33}	ε^S_{11}	ε^S_{33}
Niobate de lithium ($LiNbO_3$)	3*m*	0	0	3,7	2,5	0,2	1,3	38,9	25,7
Tantalate de lithium ($LiTaO_3$)	3*m*	0	0	2,6	1,6	$\simeq 0$	1,9	36,3	38,1
Quartz (SiO_2)	32	0,171	-0,0406	0	0	0	0	3,92	4,10
Système orthorhombique		e_{15}	e_{24}	e_{31}	e_{32}	e_{33}		ε^S_{11}	ε^S_{22}	ε^S_{33}
Niobate de baryum et de sodium ($Ba_2NaNb_5O_{15}$)	2*mm*	2,8	3,4	− 0,4	− 0,3	4,3		196	201	28

6.5 Boundary conditions

Mechanical boundary conditions

- For two rigidly bonded solids, the displacements are continuous at any point of the boundarye Σ between media M and M' : $u_i = u'_i$. Likewise, the traction is continuous: $T_{ij}\, l_j = T'_{ij}\, l_j$ with l_j the normal to Σ.
- At a free surface, displacements are unspecified but $T_{ij}\, l_j = 0$.
- At a clamped surface, stresses are unspecified but $u_i = 0$.

Electrical boundary conditions

Within the quasistatic approximation, they are similar to electrostatics.

- At an interface Σ, $\phi = \phi'$ and $E_t = E'_t$ (both the potential and the tangential electric field are continuous).
- If the surface is charged (case of a metal-dielectric interface) then $(D'_i - D_i)\; l_i = \sigma$ (σ: surface charge density). Across two dielectrics, the normal component of $\boldsymbol{D}$ is continuous.
- If the surface is short-circuited (e.g. because a metal thin-film is grounded) then $\phi = 0$.

6.6 Poynting's theorem and energy balance

Expressing the work of mechanical and electrical forces, Poynting's theorem for piezoelectric media is obtained as:

$$\frac{\mathrm{d}W}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}(E_c + E_p) + \int_\Sigma P_j \, l_j \, \mathrm{d}s \tag{20}$$

with

- kinetic energy $E_c = \int e_c \, \mathrm{d}V$ and energy density $e_c = \frac{1}{2} \rho v_i^2$
- potential energy $E_p = \int e_p \, \mathrm{d}V$ and $e_p = \frac{1}{2} (S_{ij} T_{ij} + E_k D_k)$
- Poynting's vector $P_j = -T_{ij} \, v_i + (\boldsymbol{E} \times \boldsymbol{H})_j$

As in the case of fluids, Poynting's theorem expresses the fact that work performed by internal sources in volume V is partially stored as a combination of kinetic and potential energy and partially radiated through boundary Σ. The flux of Poynting's vector accounts for this radiated power.