Lecture 4 *10-11.03.2025*

Dielectric properties of crystalline materials
- part I – symmetry and dielectric response

- Dielectric response in solids - basics

- Anisotropy of dielectric response: symmetry and Neumann principles

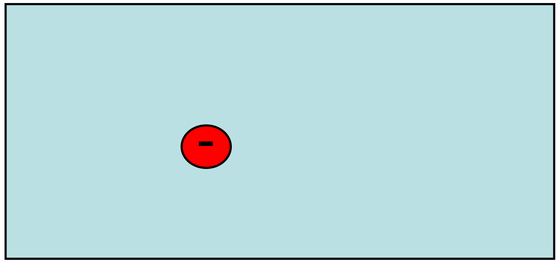
- Practical aspects of determining dielectric constant in anisotropic materials

-application-relevant practical examples)

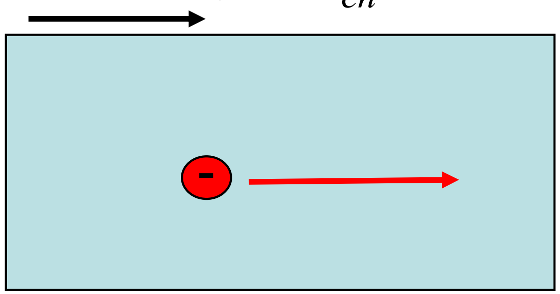
Electric response of solids

Conductivity

$E = 0 \quad < v_{ch} >= 0$



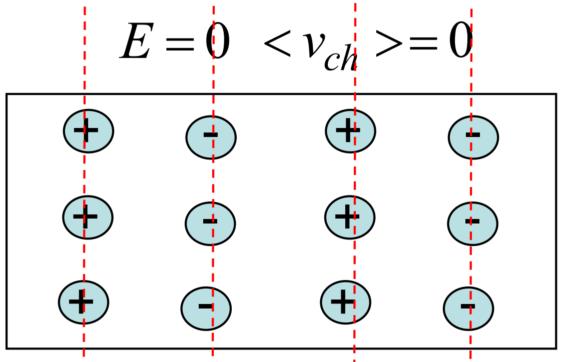
$E \neq 0 \quad < v_{ch} > \neq 0$



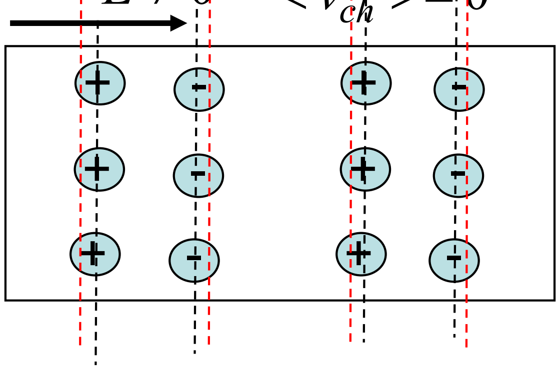
Displacements of the charges are much *larger* than the interatomic distance

Polarization

$E = 0 \quad < v_{ch} >= 0$



$E \neq 0 \quad < v_{ch} >= 0$



Displacements of the charges are much *smaller* that the interatomic distance

Electric response of solids

Conductivity

$$\vec{J} = \frac{\sum_i q_i \vec{v}_i}{V}$$

Polarization

$$\vec{P} = \frac{\sum_i q_i \delta\vec{x}_i}{V}$$

Linear response

$$J_i = \tau_{ij} E_j$$

$$P_i = \chi_{ij} E_j$$

Conductivity tensor

$$\tau_{ij}$$

Dielectric susceptibility tensor

$$\chi_{ij}$$

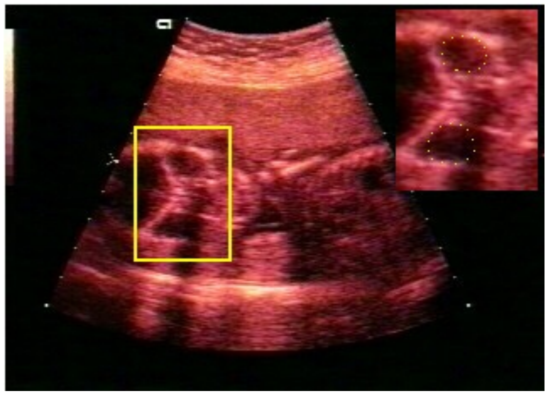
The dielectric ceramics

- Linear dielectrics
- Nonlinear dielectrics
  (e.g. ferroelectrics)

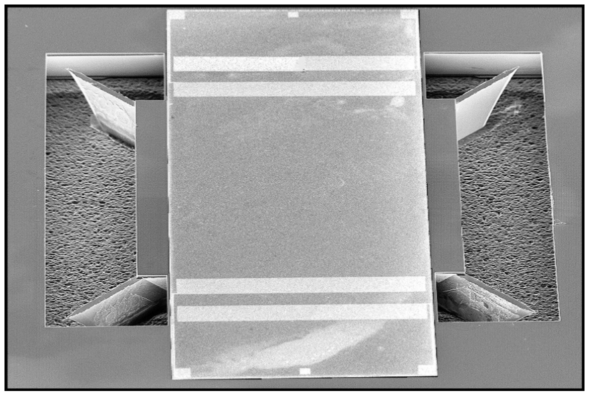
The domain of application:

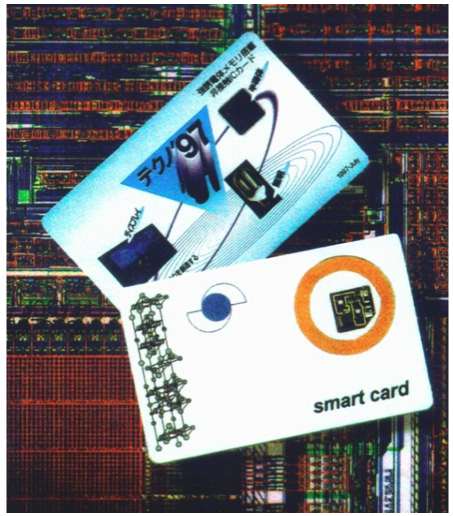
- **Communication technologies**
- **Information technologies**
- **Sensors and actuators: industrial processes, transport, protection and control of the environment, medical….**

Medical transducers:



Miniature accelerometers:



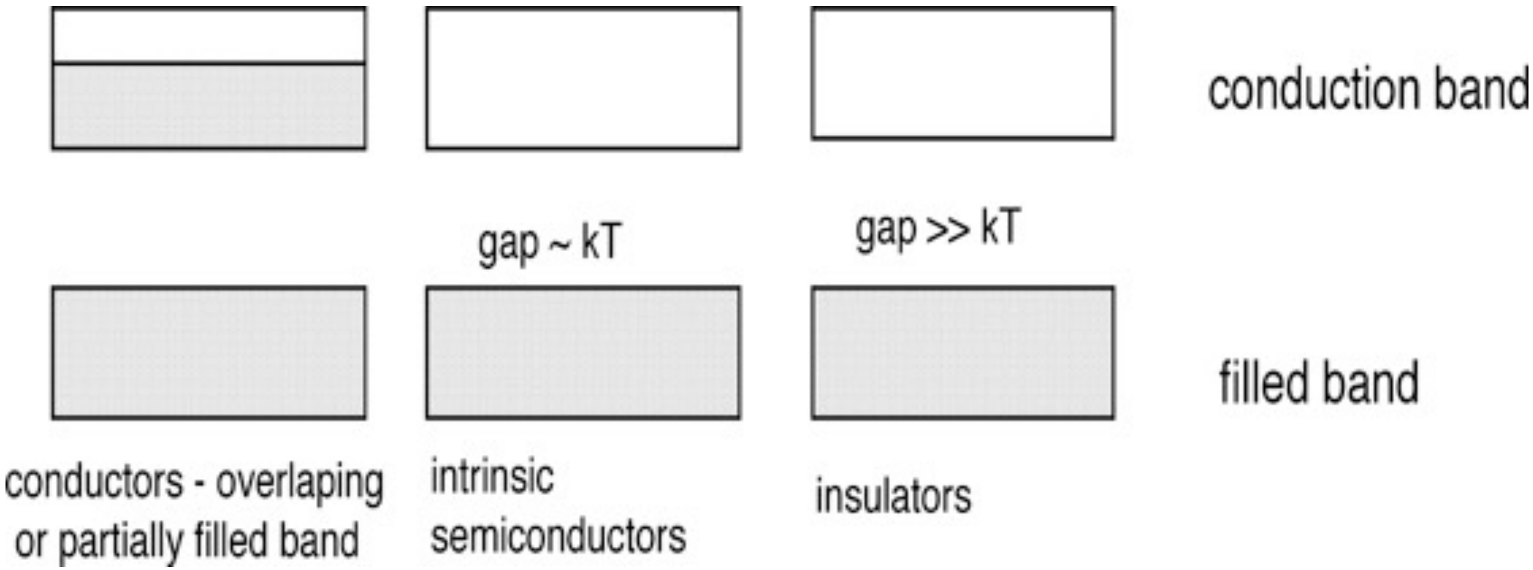


Applications of dielectric materials

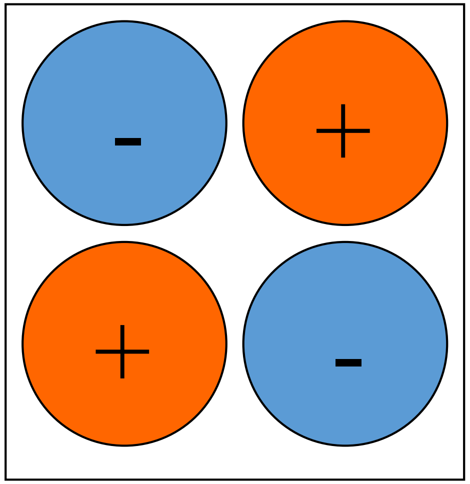
Applications	Materials(examples)
Electric insulators	porcelain
Substrates for IC	Al_2O_3, AlN
encapsulation of IC	glasses
capacitors	$BaTiO_3$
non-volatile memories	$Pb(Zr,Ti)O_3$
Piezoelectric motors and actuators	$Pb(Zr,Ti)O_3$
Ultrasonic trasnducers, resonators and filtres	$Pb(Zr,Ti)O_3$
Sensors of acceleration and pressure	SiO_2, $Pb(Zr,Ti)O_3$

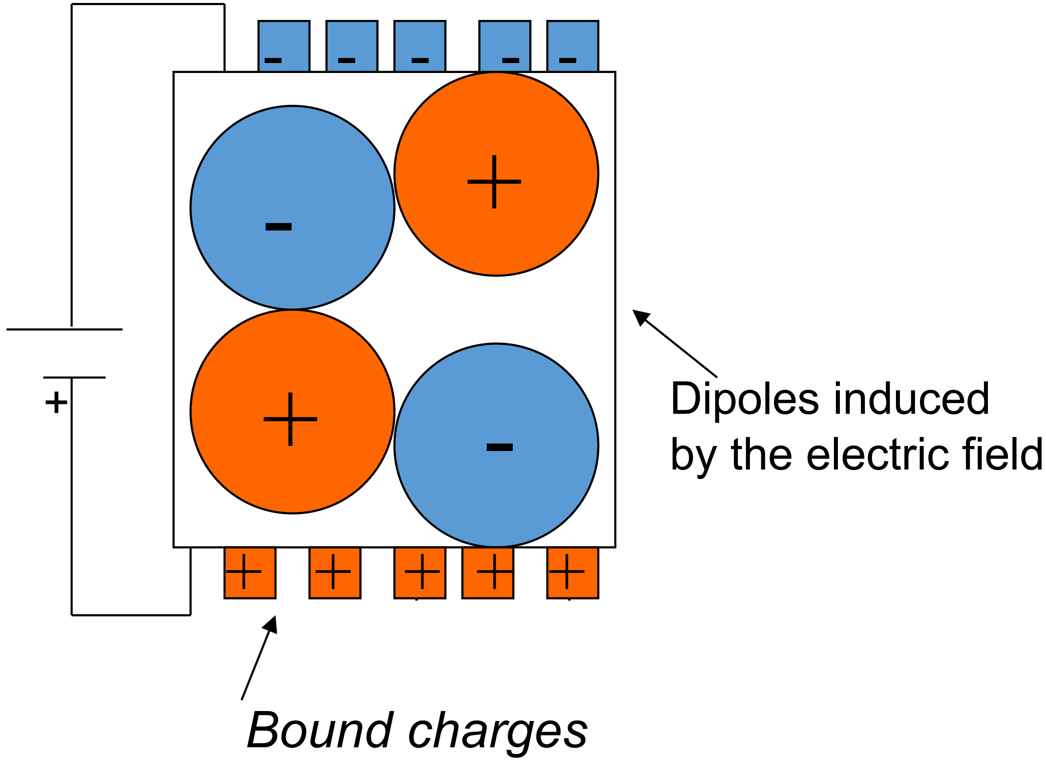
The dielectric materials (insulators)

These materials posses a relatively small number of free electrons charge carriers that can contribute to the electrical conductivity.



The dielectric materials (insulators) subjected to an electric field

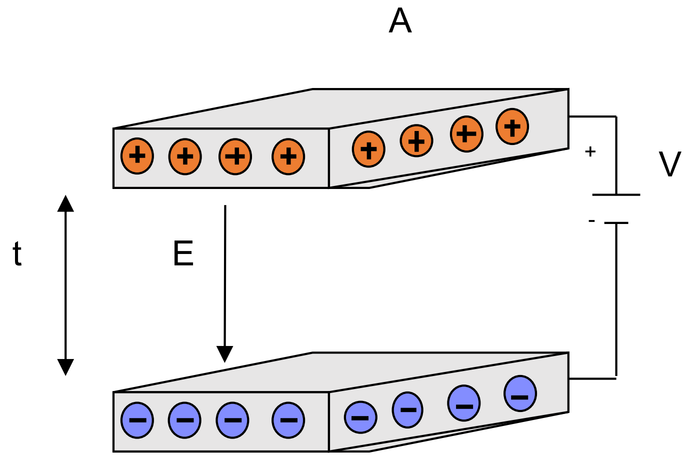




Alll charge carriers react to electric field : if they are bound, the field Induces a dipole, μ=qd

The free ends of the dipoles induced in a dielectric are neutralized by *the bound charges*

The capacitance and the dielectric constant



Capacitance between two conductors in the vacuum :

Accumulated charge : Q = C_0 V

A – electrode surface

$$C_o = \frac{\varepsilon_o A}{t} \qquad \left[F = \frac{C}{V} \right]$$

ε_o – dielectric permittivity of vacuum (electrical constant):

$\varepsilon_o = 8.85 \cdot 10^{-12}$ [Farad/m]

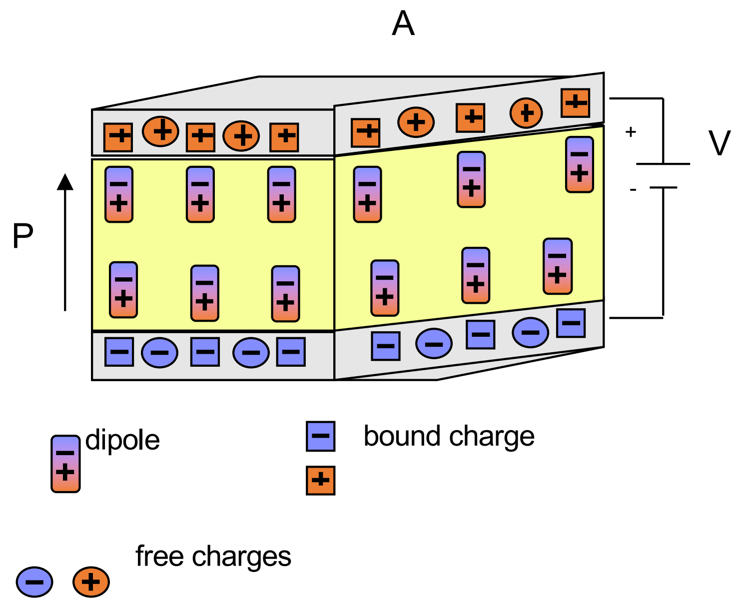
Accumulated charge :
$$Q = \frac{\varepsilon_o A}{t} V = \varepsilon_0 A E$$

Charge density :
$$D = \frac{Q}{A} = \varepsilon_0 E \quad [C/m^2]$$

The capacitance and the dielectric constant

Capacitance between two conducting plates with a dielectric :

Addition of charges bound to dipoles induced by the polarization of the material



Accumulated charge :

$$Q_{tot} = Q_0 + Q_b$$

free bound

$$Q_{tot} = k\, C_0\, V \qquad C = k\, C_0$$

$$C = k\, \varepsilon_o \frac{A}{t} = \varepsilon \frac{A}{t}\, [F]$$

k – relative dielectric constant of the material

$\varepsilon = k\, \varepsilon_o$ – absolute permittivity of the material [F/m]

Dielectric response

$$P_i = \chi_{ij} E_j$$

or

$$D_i = \varepsilon_o E_i + P_i \qquad D_i = \varepsilon_0 K_{ij} E_j \qquad \varepsilon_0 K_{ij} = \varepsilon_0 \delta_{ij} + \chi_{ij}$$

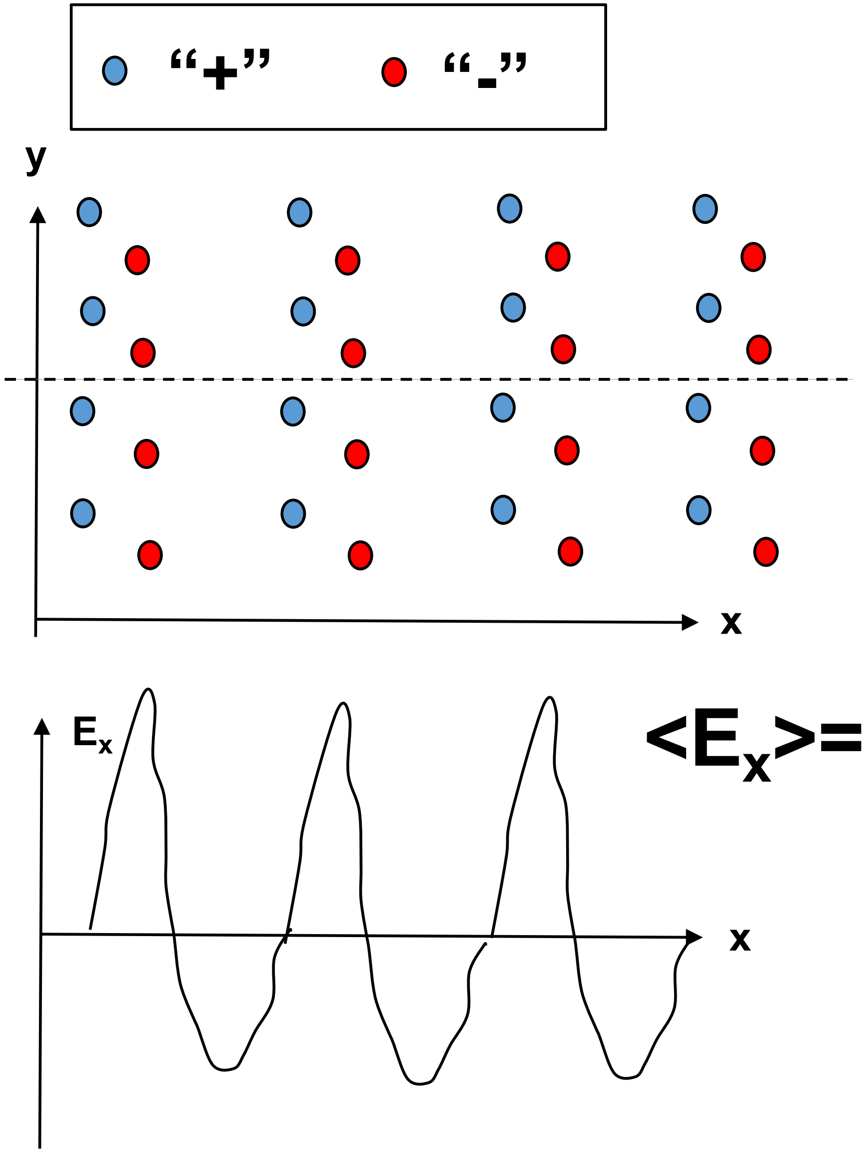
in vacuum $\quad P_i = 0 \qquad D_i = \varepsilon_0 E_i \qquad K_{ij} = \delta_{ij}$

Internal symmetry $\longrightarrow$ $\boxed{K_{ij} = K_{ji}}$

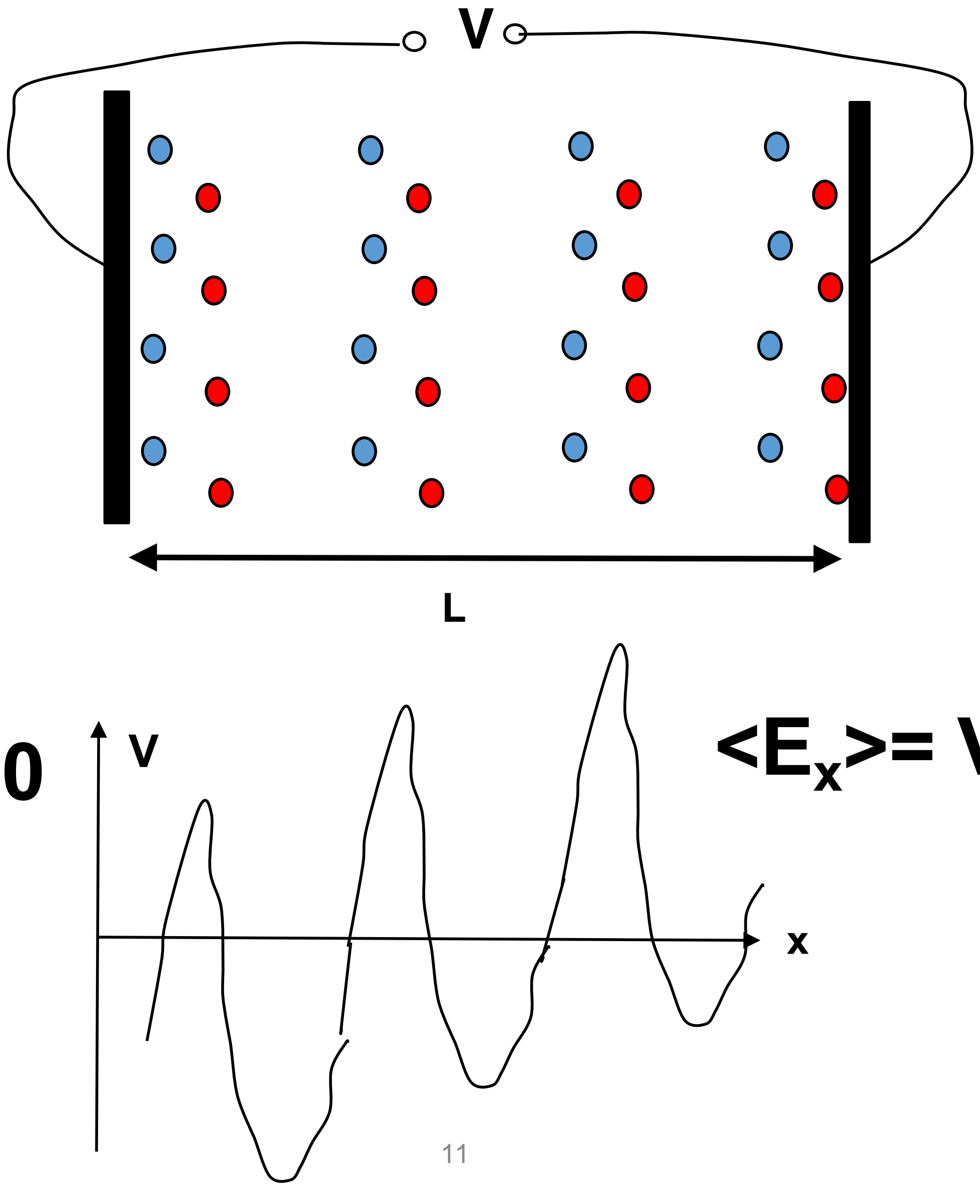
Dielectric permittivity tensor is a symmetric second rank tensor

(why symmetric – will be shown later based on thermodynamics)

How to measure and control macroscopic electric field ?

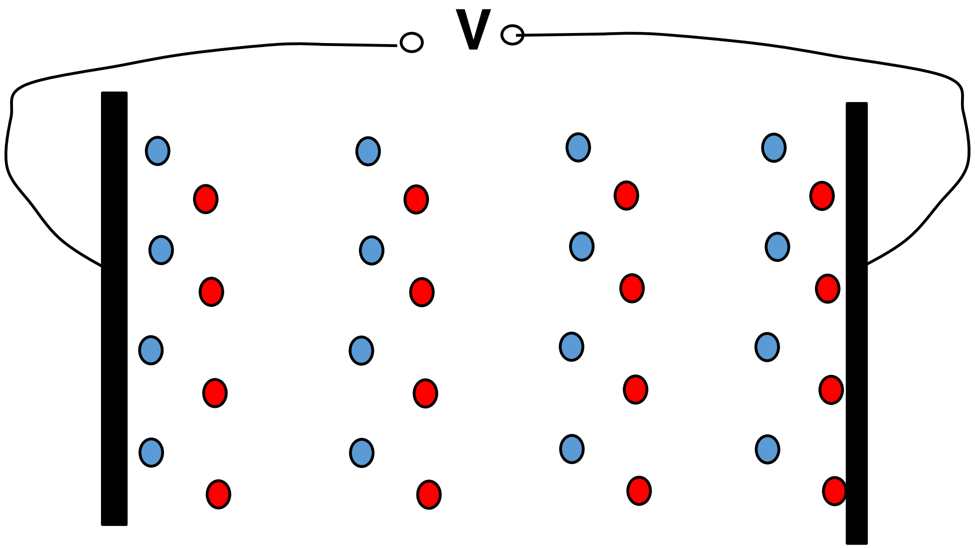


$\langle E_x \rangle = 0$



$\langle E_x \rangle = V/L$

Macroscopic electric field



$$\vec{E} = \vec{E}_{\text{loc}} + \vec{E}_{\text{mac}}$$

$$\vec{E}_{\text{mac}}(\vec{r}) = \frac{1}{V}\int \vec{E}dV$$

Integration over a small but macroscopic

(containing many atoms)

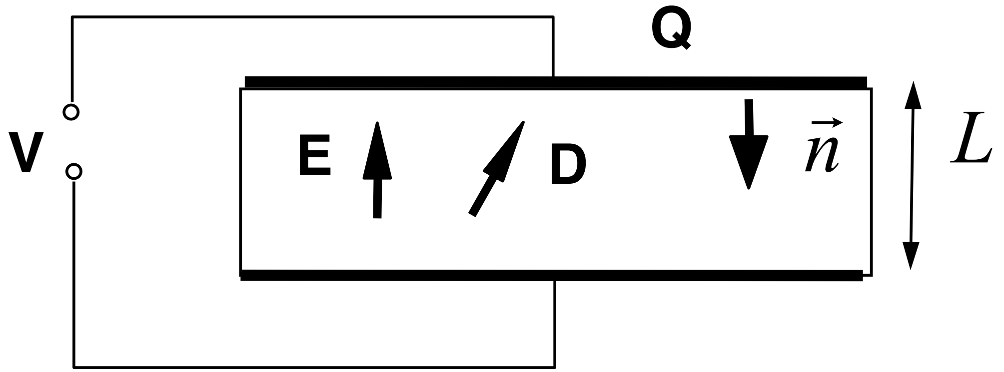
volume around $\vec{r}$.

- Macroscopic field is always normal to the metal in contact.

- Further in the course "field" = "macroscopic field"

$$\vec{E}_{\text{mac}} \Rightarrow \vec{E}$$

How to measure and control macroscopic electrical displacemnet?



$\vec{E} \uparrow\uparrow \vec{n}$ $\qquad |V| = L|\vec{E}|$

$\vec{n}$ – outer normal to the metal

MEASURED

TO CALCULATE DISPLACEMENT

S – electrode area

Q – charge on the metal

$$\frac{Q}{S} = D_i n_i$$

This follows from Maxwell equations $\quad \mathrm{div}\vec{D} = \rho_{\mathrm{free}}$

Neumann principle

Any tensor describing a physical property of a material should not be affected when one changes the reference frame according to the symmetry elements of the material

Should be invariant with respect to the symmetry elements of the material!

Neumann principle

$$K_{i'j'} = a_{i'i}(t_1)a_{j'j}(t_1)K_{ij}$$

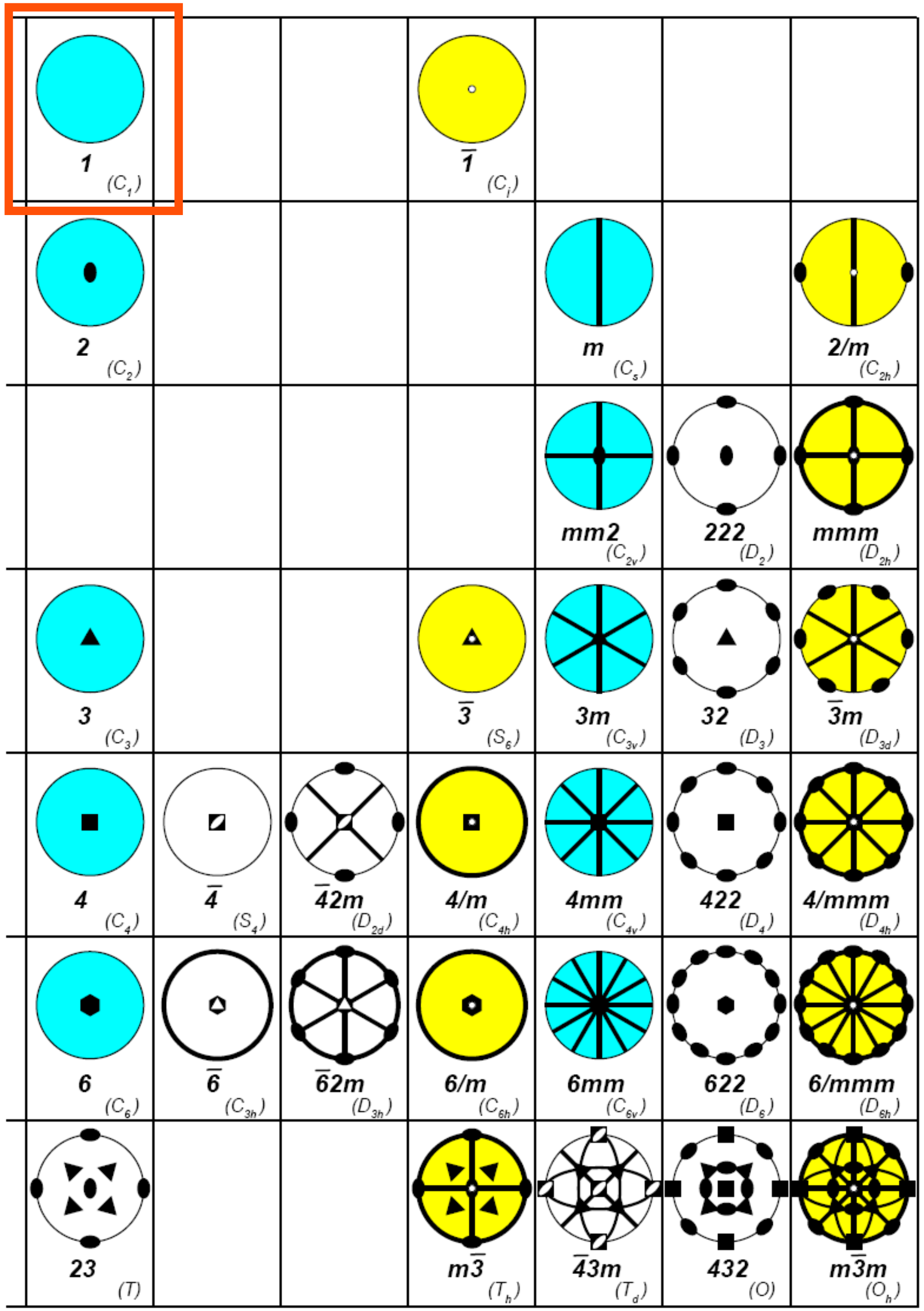
$$K_{i'j'} = a_{i'i}(t_2)a_{j'j}(t_2)K_{ij}$$

$$K_{i'j'} = a_{i'i}(t_3)a_{j'j}(t_3)K_{ij}$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdot$$

$$K_{i'j'} = a_{i'i}(t_n)a_{j'j}(t_n)K_{ij}$$

$t_1, t_2, t_3 \ldots\ldots t_n$ **- symmetry elements of the material**



1

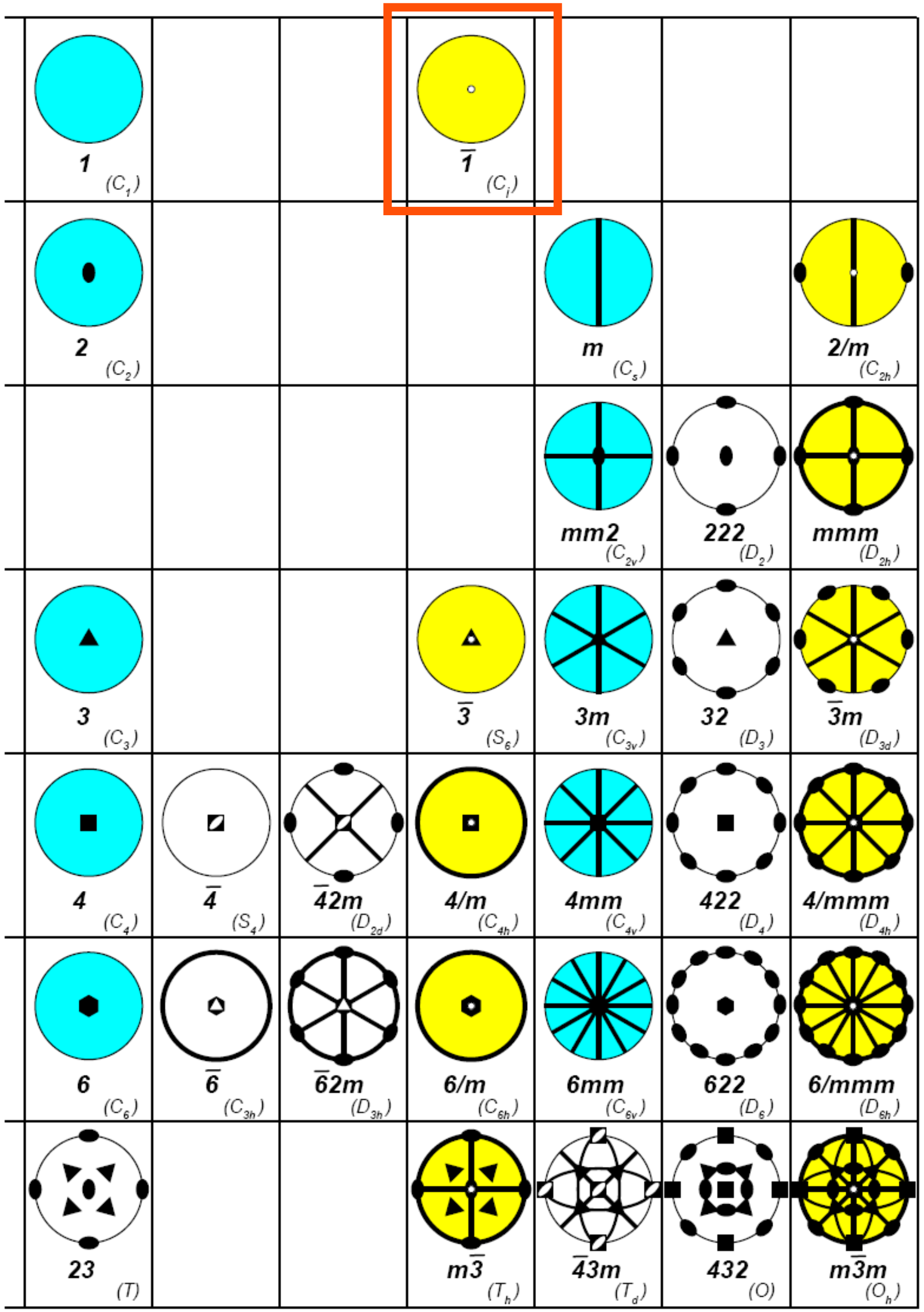
No symmetry elements

No Neumann equations

No restrictions

$$\begin{pmatrix} K_{11} & K_{12} & K_{13} \\ & K_{22} & K_{23} \\ & & K_{33} \end{pmatrix}$$

6 independent components



$$\bar{1}$$

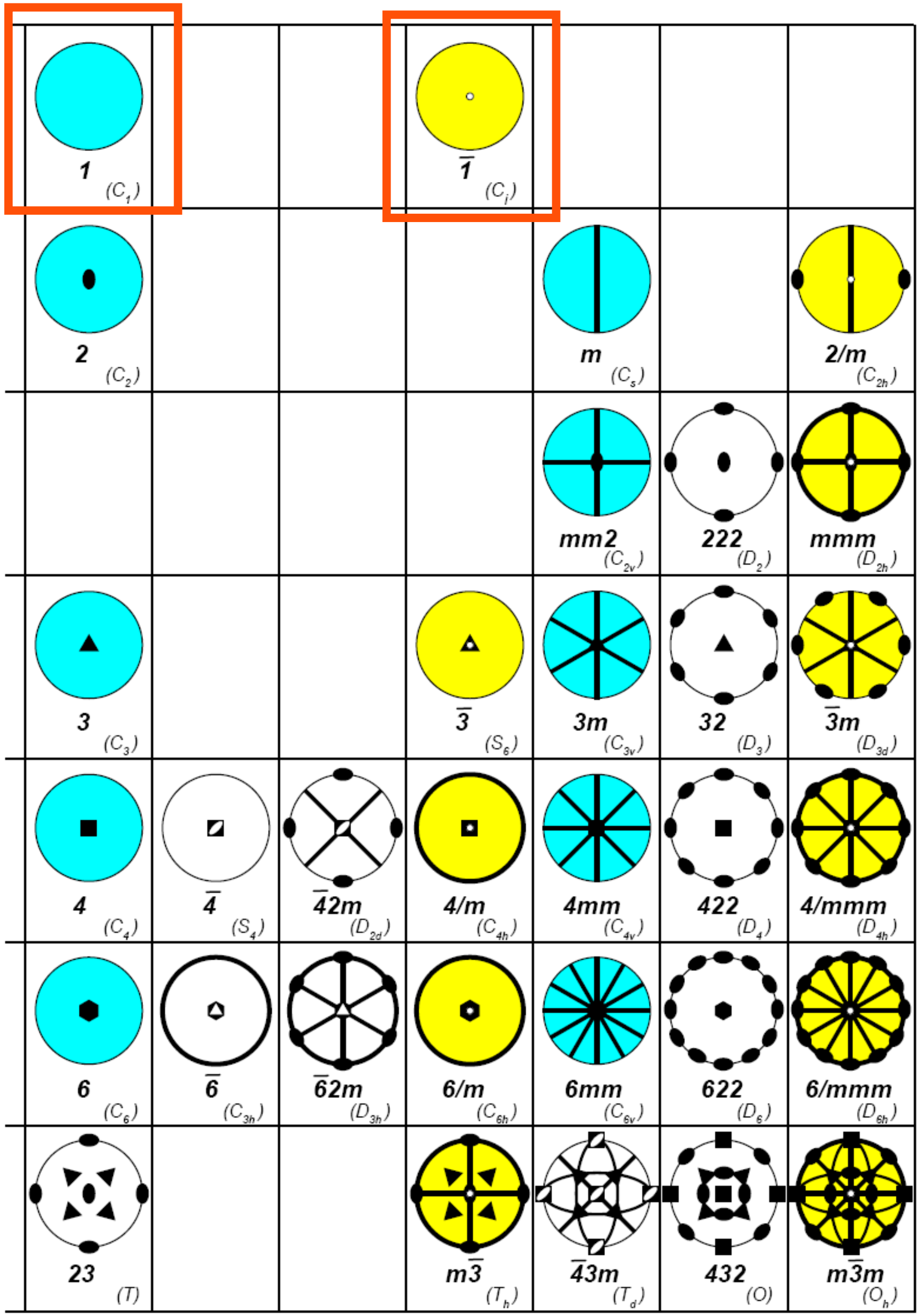
1 symmetry element
-inversion

1 Neumann equation

$$K_{i'j'} = a_{i'i} a_{j'j} K_{ij}$$

$$a_{ij} = -\delta_{ij}$$

Still no restrictions!



Material symmetry

1 and $\bar{1}$

Studied property = dielectric response

Property symmetry

at least $\bar{1}$

Property symmetry is higher than material symmetry

Symmetry of a tensor or symmetric tensor: avoiding confusion

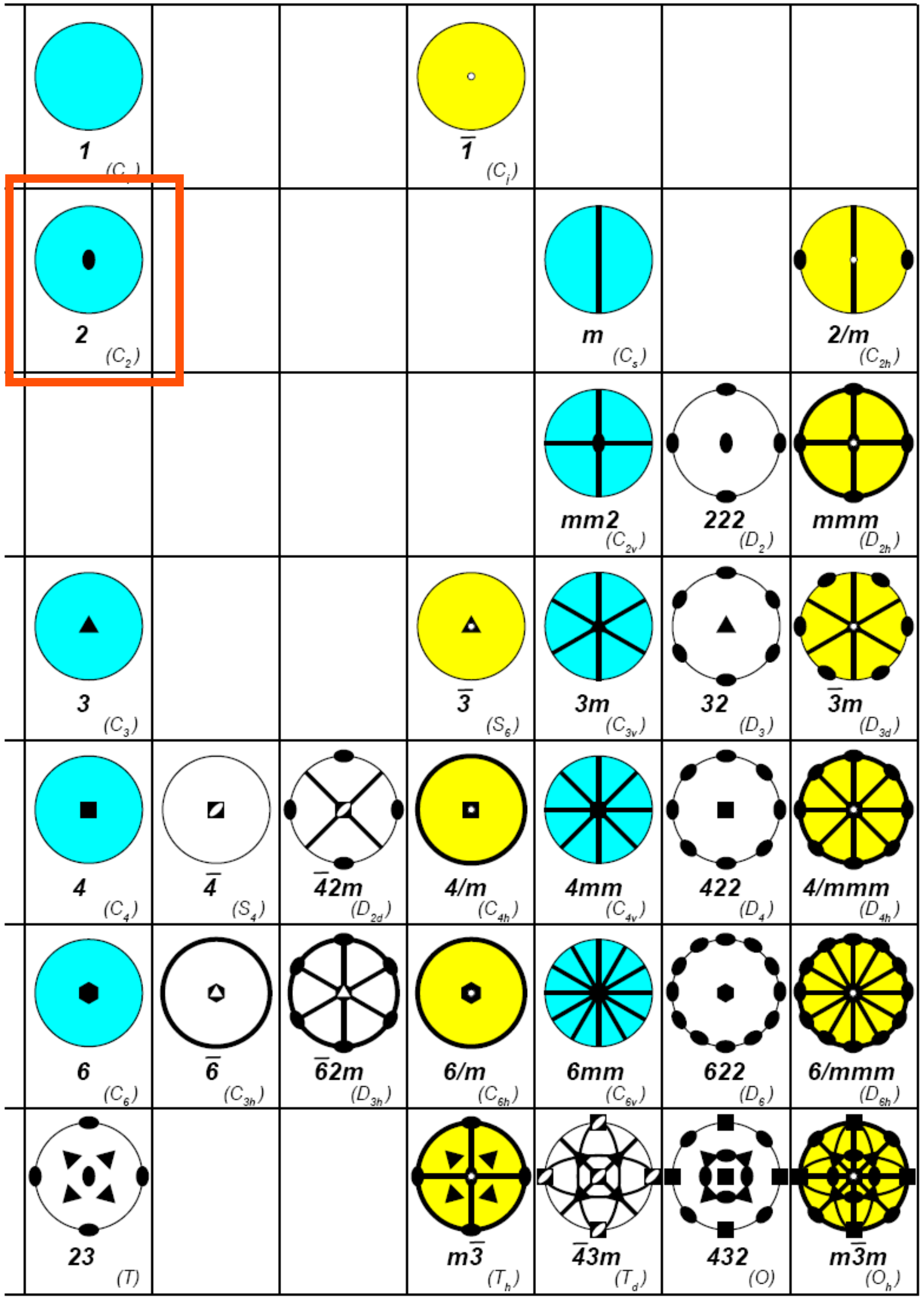
Attention: possible terminological confusion !

(i) Symmetric second rank tensor (permutational symmetry)

$$K_{ij} = K_{ji}$$

(ii) The symmetry of K_{ij} with respect to a change of the reference frame = **the symmetry of the property**

$$K_{ij} = a_{is} a_{jt} K_{st}$$



2

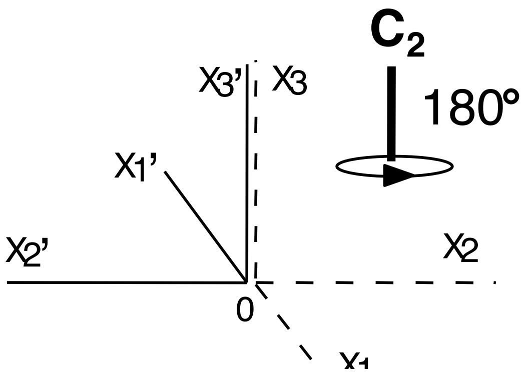
1 symmetry element
-180^0-rotation

1 Neumann equation

$$K_{i'j'} = a_{i'i} a_{j'j} K_{ij}$$

$$a_{ij} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Getting Neumann equation



$$p'_3 = p_3$$
$$p'_2 = -p_2$$
$$p'_1 = -p_1$$

$$p'_1 p'_1 = p_1 p_1 \Rightarrow K'_{11} = K_{11}$$
$$p'_1 p'_2 = p_1 p_2 \Rightarrow K'_{12} = K_{12}$$
$$p'_1 p'_3 = -p_1 p_3 \Rightarrow K'_{13} = -K_{13}$$

*Here some simplification is possible: instead of two vectors **p** and **q**, just use two times the same vector **p** – works for a symmetric tensor*

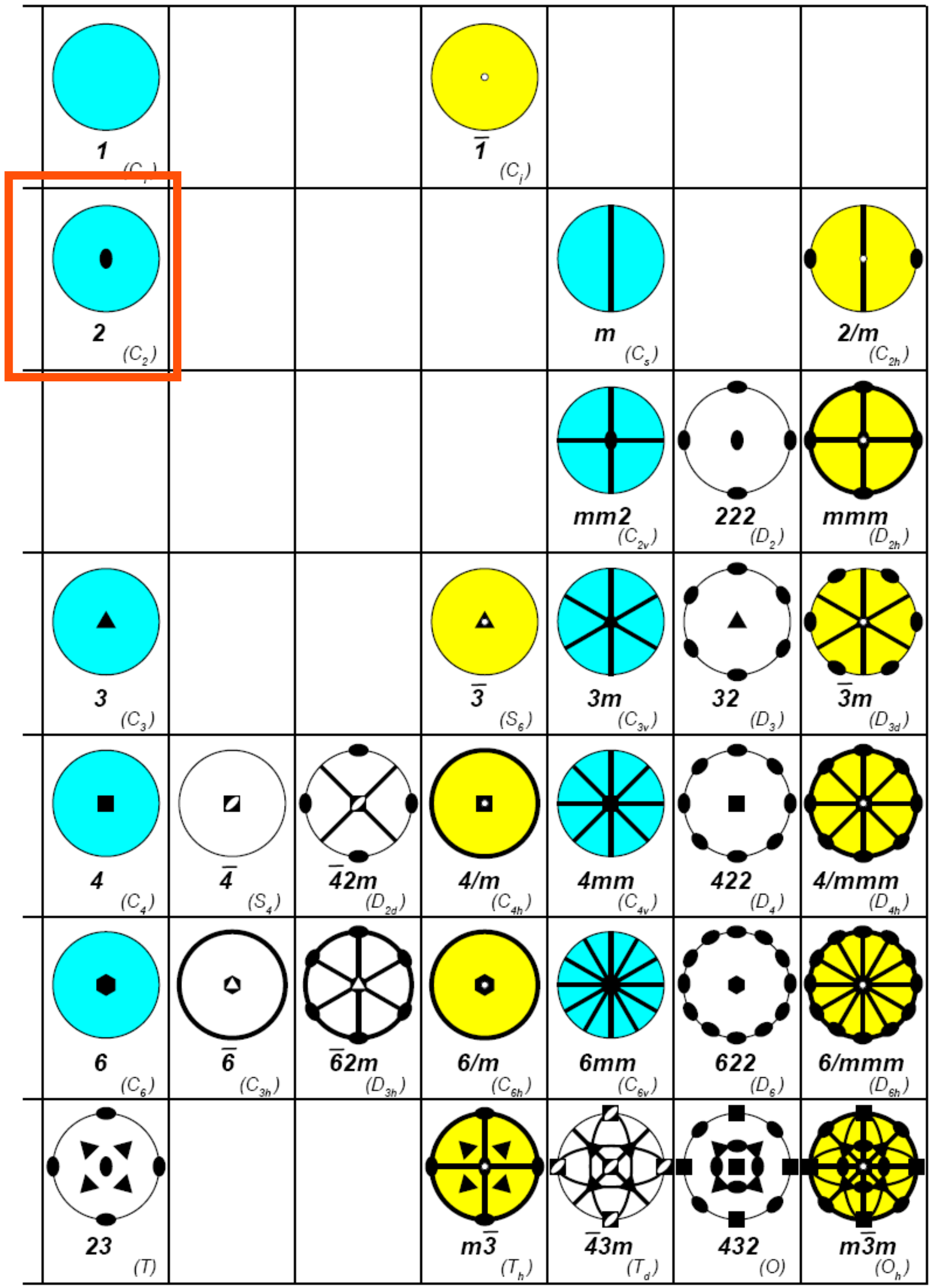
(i) Transformation

$$K'_{ij} = \begin{pmatrix} K_{11} & K_{12} & -K_{13} \\ & K_{22} & -K_{23} \\ & & K_{33} \end{pmatrix}$$

(ii) Neumann equation

Old frame New frame

$$\begin{pmatrix} K_{11} & K_{12} & K_{13} \\ & K_{22} & K_{23} \\ & & K_{33} \end{pmatrix} = \begin{pmatrix} K_{11} & K_{12} & -K_{13} \\ & K_{22} & -K_{23} \\ & & K_{33} \end{pmatrix}$$



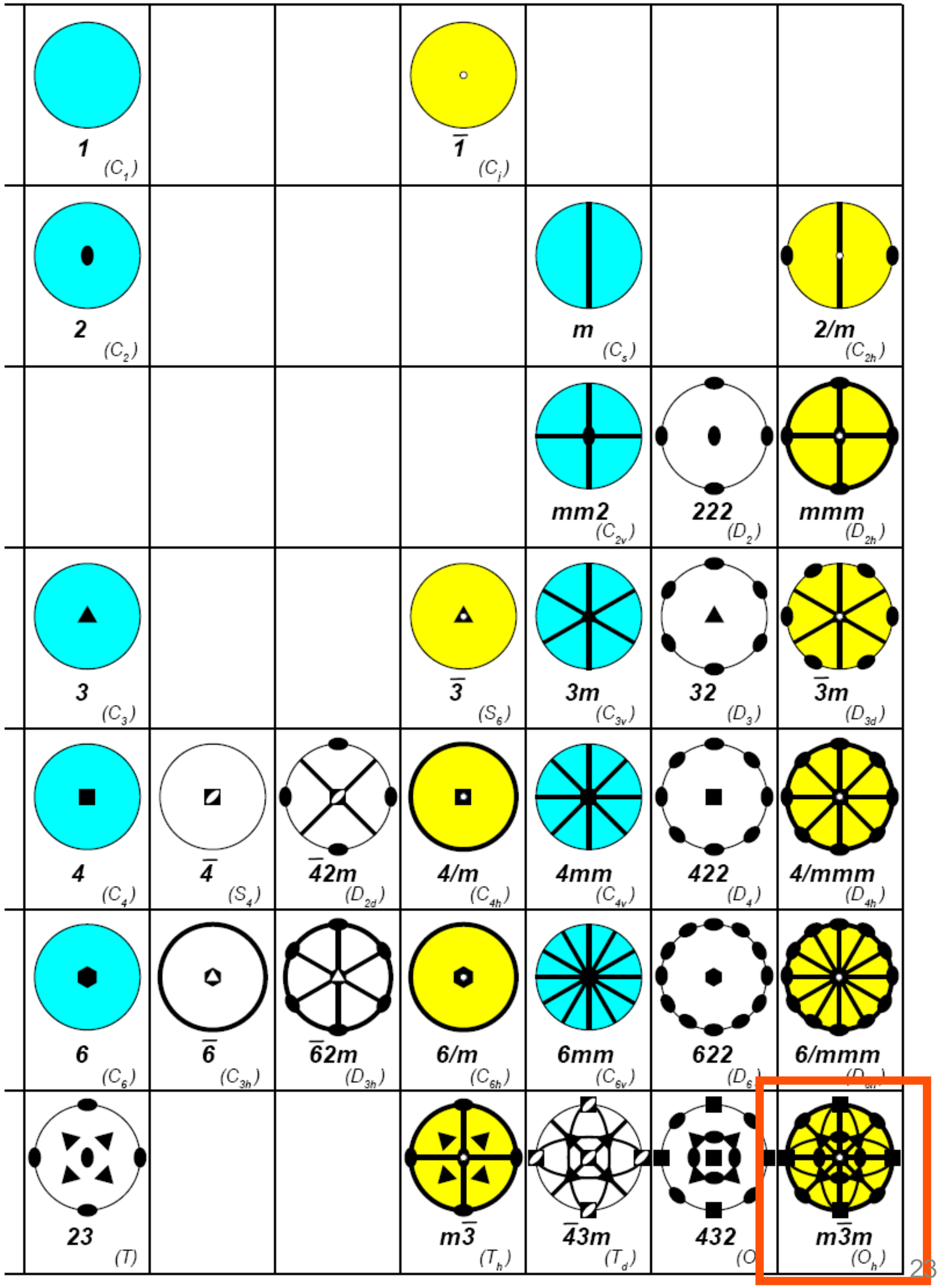
2

Neumann equation

$$\begin{pmatrix} K_{11} & K_{12} & K_{13} \\ & K_{22} & K_{23} \\ & & K_{33} \end{pmatrix} = \begin{pmatrix} K_{11} & K_{12} & -K_{13} \\ & K_{22} & -K_{23} \\ & & K_{33} \end{pmatrix}$$

4 independent components

$$\begin{pmatrix} K_{11} & K_{12} & 0 \\ & K_{22} & 0 \\ & & K_{33} \end{pmatrix}$$



$m\bar{3}m$

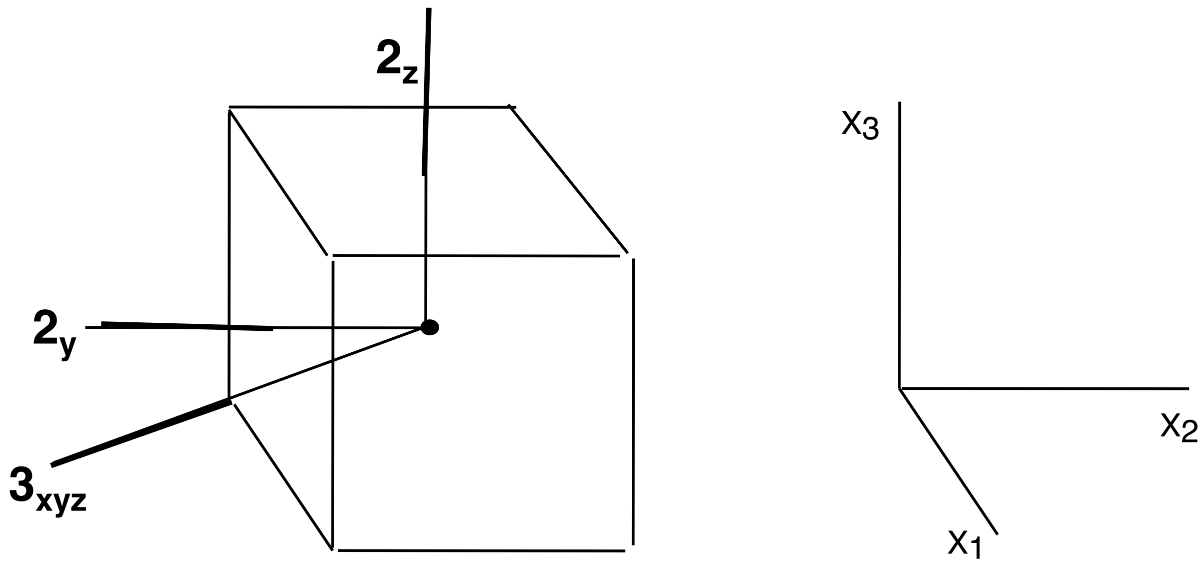
47 symmetry elements

47 Neumann equations

$$K_{i'j'} = a_{i'i}a_{j'j}K_{ij}$$

3 Neumann equations

$m\bar{3}m$



(t$_1$)

2_z

$$p_1' = -p_1$$
$$p_2' = -p_2$$
$$p_3' = p_3$$

(t$_2$)

2_y

$$p_1' = -p_1$$
$$p_2' = p_2$$
$$p_3' = -p_3$$

(t$_3$)

3_{xyz}

$$p_1' = p_3$$
$$p_2' = p_1$$
$$p_3' = p_2$$

3 Neumann equations

$m\bar{3}m$

$$\begin{pmatrix} K_{11} & K_{12} & K_{13} \\ & K_{22} & K_{23} \\ & & K_{33} \end{pmatrix} \xRightarrow{\mathbf{2_z}} \begin{pmatrix} K_{11} & K_{12} & 0 \\ & K_{22} & 0 \\ & & K_{33} \end{pmatrix}$$

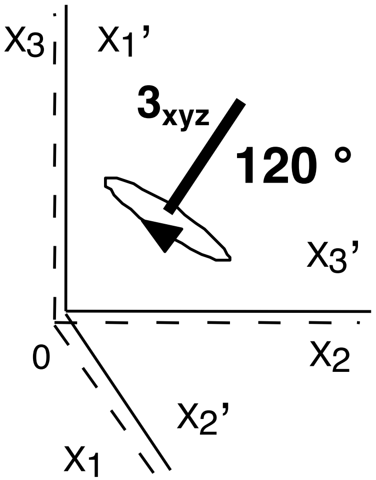
$$\begin{pmatrix} K_{11} & K_{12} & 0 \\ & K_{22} & 0 \\ & & K_{33} \end{pmatrix} \xRightarrow{\mathbf{2_y}} \begin{pmatrix} K_{11} & 0 & 0 \\ & K_{22} & 0 \\ & & K_{33} \end{pmatrix}$$

3 Neumann equations

$m\bar{3}m$

$$\begin{pmatrix} K_{11} & 0 & 0 \\ & K_{22} & 0 \\ & & K_{33} \end{pmatrix} \overset{3_{xyz}}{\Longrightarrow} \begin{pmatrix} K & 0 & 0 \\ & K & 0 \\ & & K \end{pmatrix}$$

Type equation here.



$$p'_1 = p_3$$
$$p'_2 = p_1$$
$$p'_3 = p_2$$

$$p'_1\, p'_1 = p_3 p_3 \Rightarrow K'_{11} = K_{33}$$
$$p'_2\, p'_2 = p_1 p_1 \Rightarrow K'_{22} = K_{11}$$
$$p'_3\, p'_3 = p_2 p_2 \Rightarrow K'_{33} = K_{22}$$

$$K_{22} = K_{33} = K_{11} = K$$

44 Neumann equations

$m\bar{3}m$

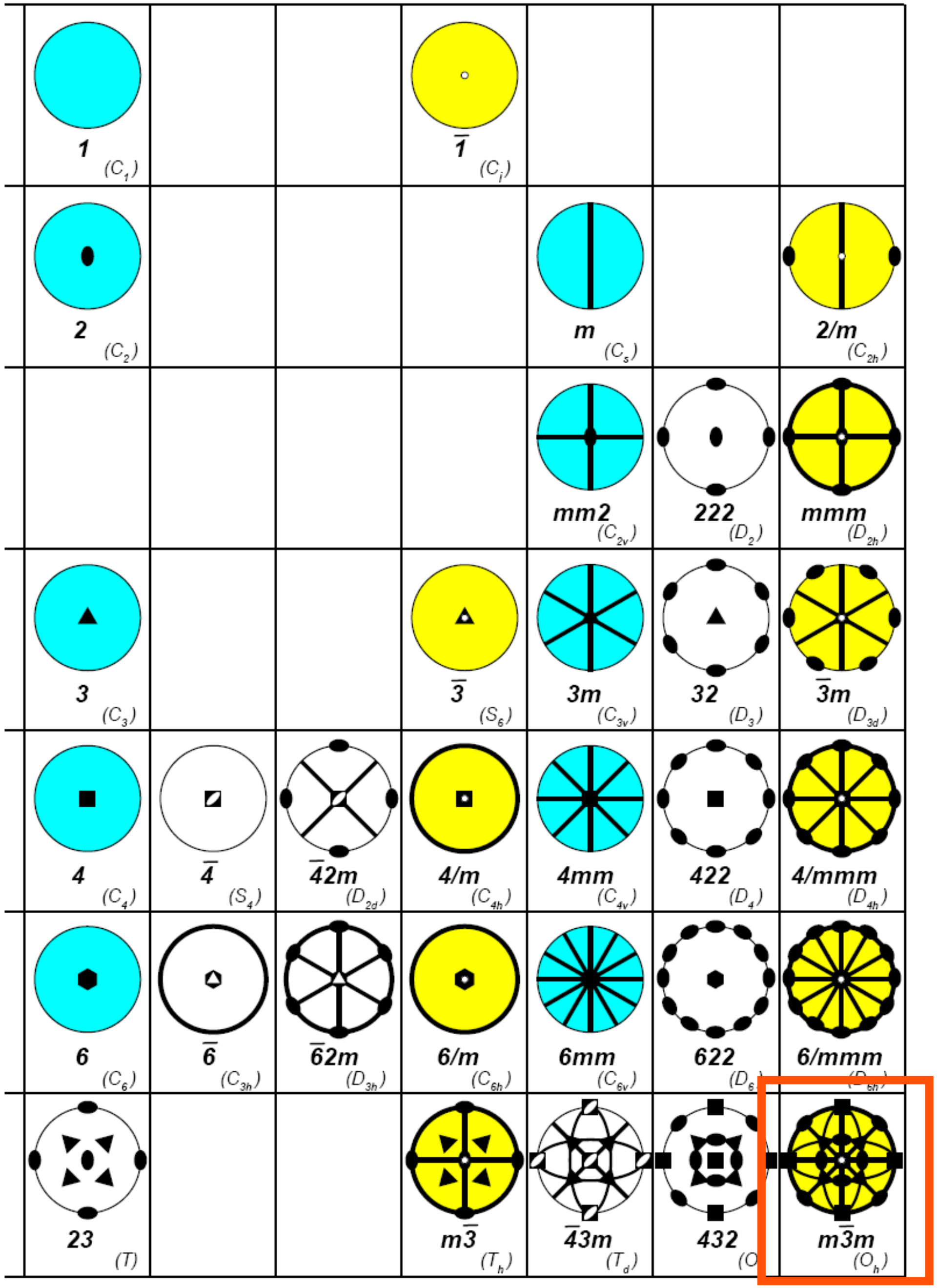
47-3 = 44

$$K_{i'j'} = a_{i'i}(t_1)a_{j'j}(t_1)K_{ij}$$
$$K_{i'j'} = a_{i'i}(t_2)a_{j'j}(t_2)K_{ij}$$
$$K_{i'j'} = a_{i'i}(t_3)a_{j'j}(t_3)K_{ij}$$
$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$
$$K_{i'j'} = a_{i'i}(t_n)a_{j'j}(t_n)K_{ij}$$

$$K_{ij} = K\delta_{ij} = \begin{pmatrix} K & 0 & 0 \\ & K & 0 \\ & & K \end{pmatrix}$$

Kronecker delta
is an invariant tensor

No further restrictions!



$m\bar{3}m$

47 Neumann equations

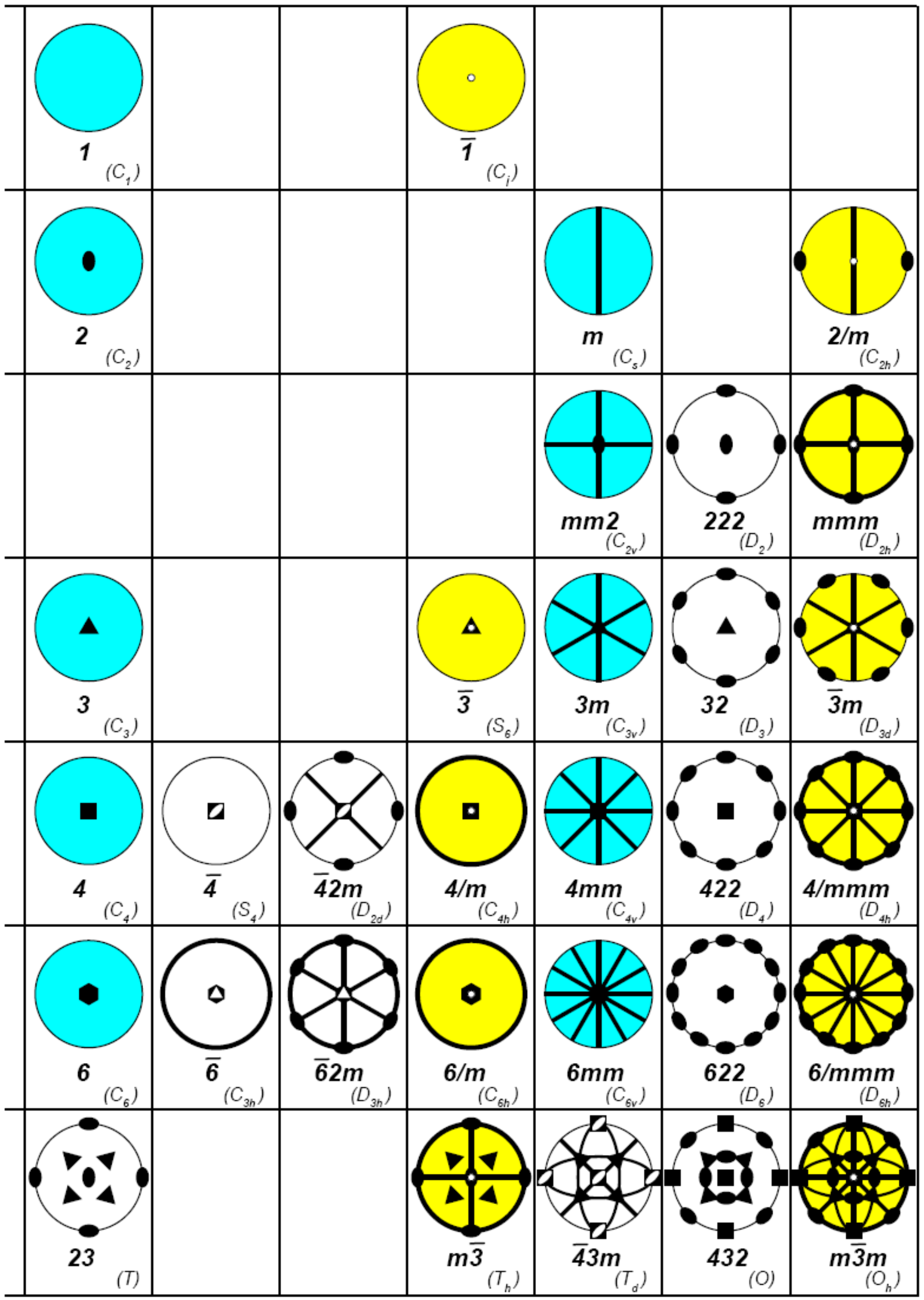
$$K_{ij} = K\delta_{ij} = \begin{pmatrix} K & 0 & 0 \\ & K & 0 \\ & & K \end{pmatrix}$$

1 independent component

Actual symmetry of the property

$\infty\infty m$

5 structures of K-tensor



$$\begin{pmatrix} K_{11} & K_{12} & K_{13} \\ & K_{22} & K_{23} \\ & & K_{33} \end{pmatrix}$$

$$\begin{pmatrix} K_{11} & 0 & K_{13} \\ & K_{22} & 0 \\ & & K_{33} \end{pmatrix}$$

$$\begin{pmatrix} K_{11} & 0 & 0 \\ & K_{22} & 0 \\ & & K_{33} \end{pmatrix}$$

$$\begin{pmatrix} K_1 & 0 & 0 \\ & K_1 & 0 \\ & & K_3 \end{pmatrix}$$

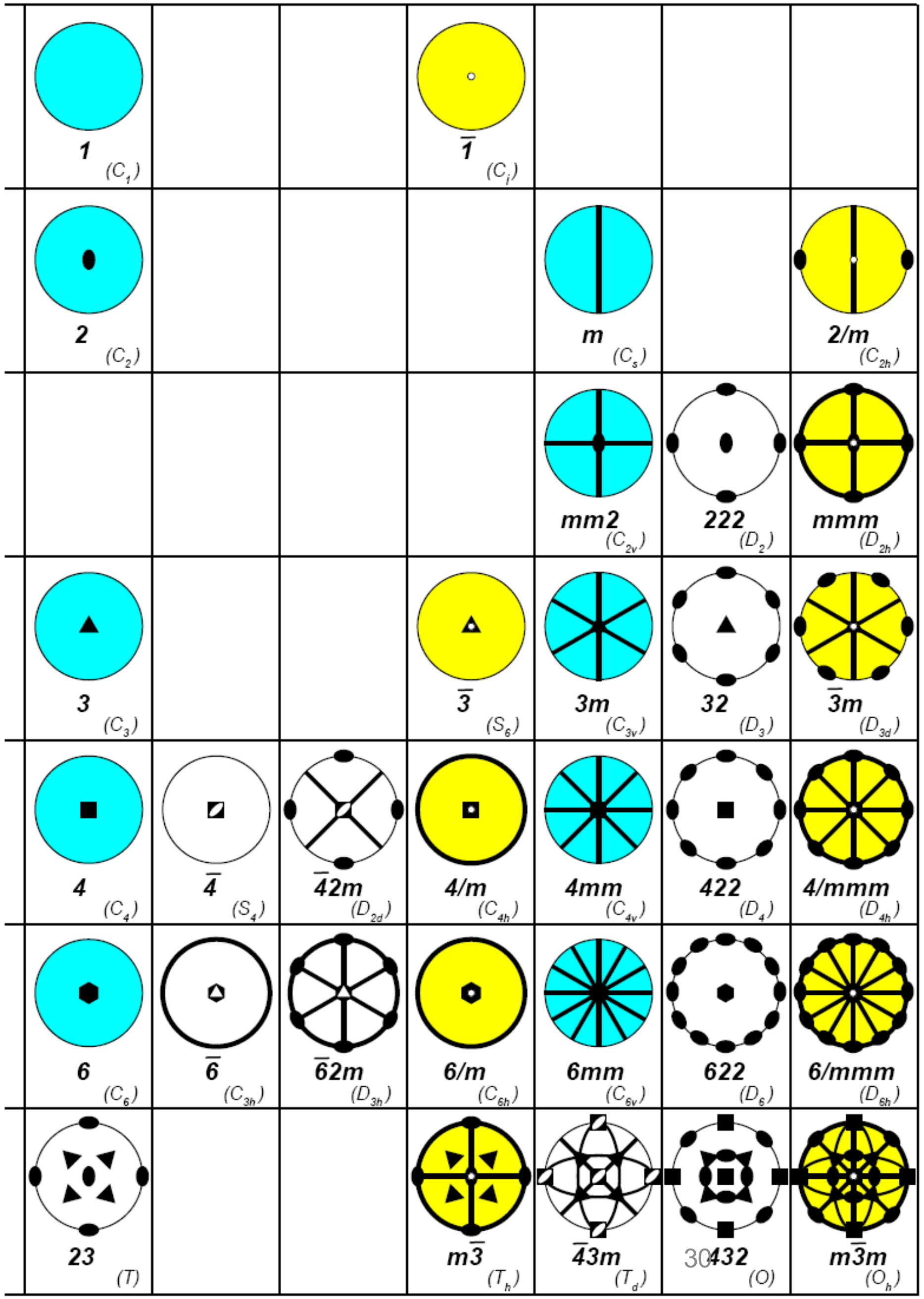
$\infty \quad \infty m \quad \infty 2$

$\infty / m \quad \infty / mm$

$$\begin{pmatrix} K & 0 & 0 \\ & K & 0 \\ & & K \end{pmatrix}$$

$\infty\infty \quad \infty\infty m$

Conventional choice of axes

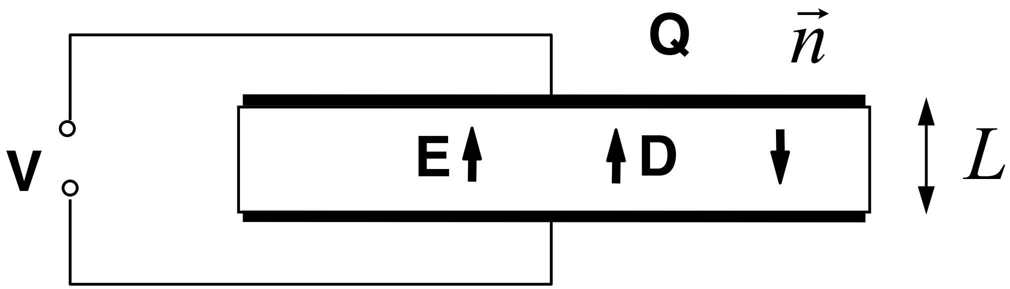


Triclinic	**arbitrary**
Monoclinic	$2,\bar{2} \parallel X_2$
Orthorhombic	**The axes are parallel to 2-fold axes; in *mm2* -** $2 \parallel X_3$
Trigonal	$3 \parallel X_3$
Tetragonal	$4,\bar{4} \parallel X_3$
Hexagonal	$6,\bar{6} \parallel X_3$
Cubic	**The axes are parallel to the edges of the cube**

Anisotropy of dielectric response

vacuum

$$K_{ij} = \delta_{ij} \qquad D_i = \varepsilon_o E_i$$



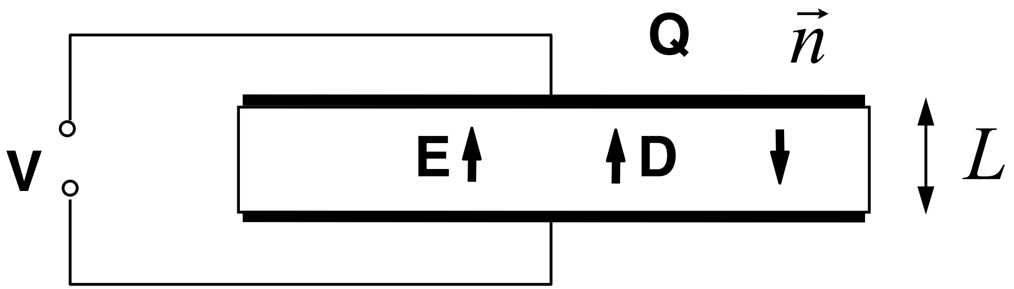
S – electrode area

$$C = \frac{Q}{V} \qquad Q = SD_i n_i \qquad E_i = n_i \frac{V}{L}$$

Dielectric response of vacuum is isotropic

$$D_i = \varepsilon_o E_i \qquad \vec{E} \uparrow\uparrow \vec{n} \qquad C_0 = \frac{Q}{V} = \frac{S\varepsilon_0 E}{LE} = \frac{\varepsilon_0 S}{L}$$

Anisotropy of dielectric response



S – electrode area

isotropic dielectric

$$K_{ij} = K\delta_{ij}$$

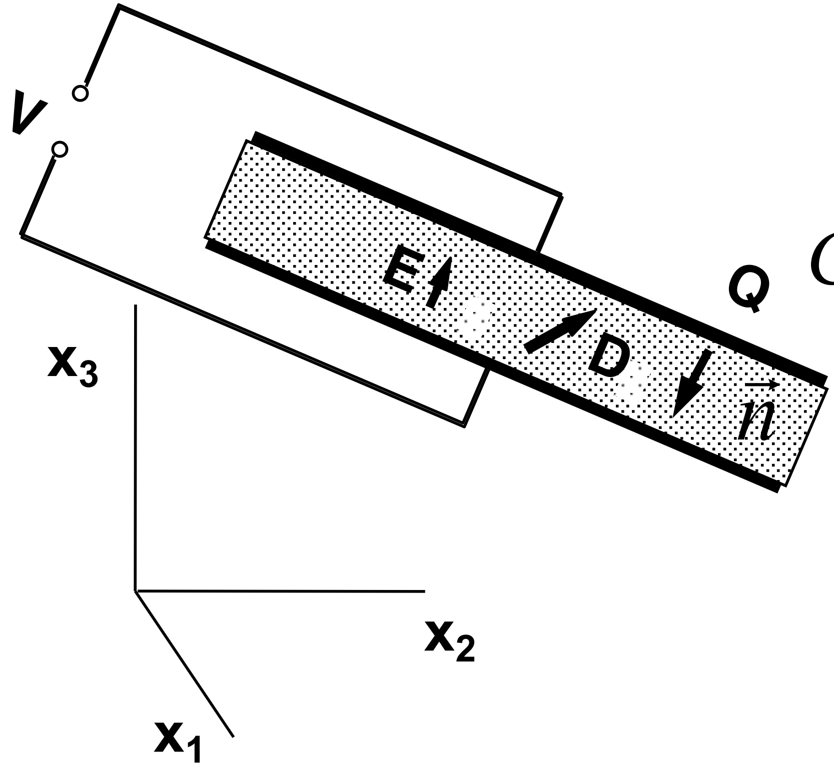
$$D_i = \varepsilon_o K E_i$$

$$C = \frac{Q}{V} \qquad Q = S D_i n_i \qquad E_i = n_i \frac{V}{L}$$

$$C_{diel} = \frac{Q}{V} = \frac{S\varepsilon_0 K E}{LE} = \frac{\varepsilon_0 K S}{L} \qquad \frac{C_{diel}}{C_0} = K$$

Dielectric constant

Anisotropy of dielectric response *reminder*



Reference frame
associated with the material

anisotropic dielectric K_{ij}

$$C_{diel} = \frac{Q}{V} = \frac{Sn_i \boxed{\varepsilon_0 K_{ij} n_j E}}{LE} = C_0 \times n_i K_{ij} n_j$$

$$\boxed{D_i}$$

In the principal axes

$$K_{eff}(\vec{n}) = n_1^2 K^{(1)} + n_2^2 K^{(2)} + n_3^2 K^{(3)}$$

Dielectric response is anisotropic

Anisotropy of dielectric response

Anisotropy of dielectric response is controlled by the shape of the dependence

$$K_{eff}(\vec{n}) = \frac{C_{diel}}{C_0} = n_i K_{ij} n_j$$

Effective dielectric constant

n_j controls the way the plate is cut from the material !

In the principal axes

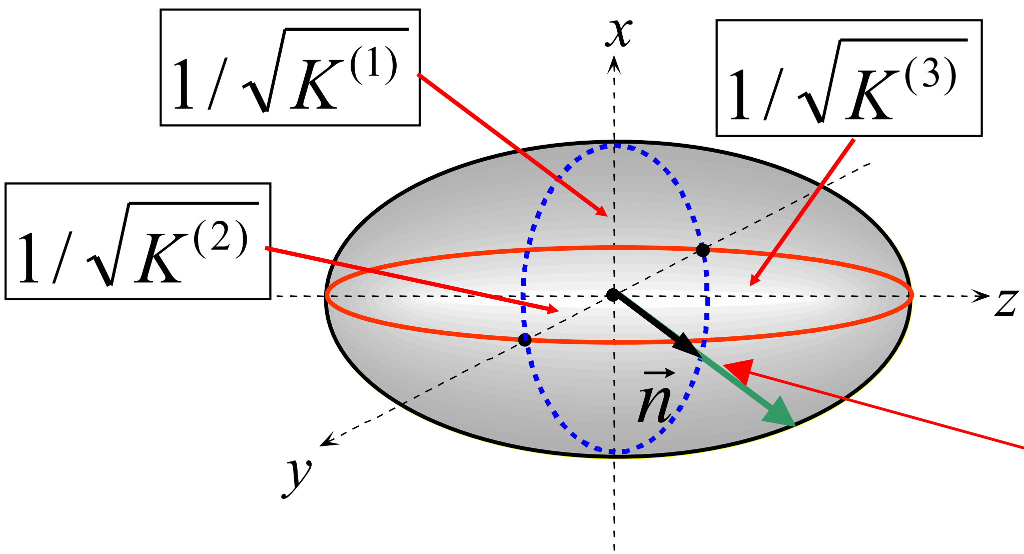
$$K_{eff}(\vec{n}) = n_1^2 K^{(1)} + n_2^2 K^{(2)} + n_3^2 K^{(3)}$$

Visualization of dielectric anisotropy

$$K_{ij}X_iX_j = 1$$

"Representation quadric"

In principle axes of the tensor



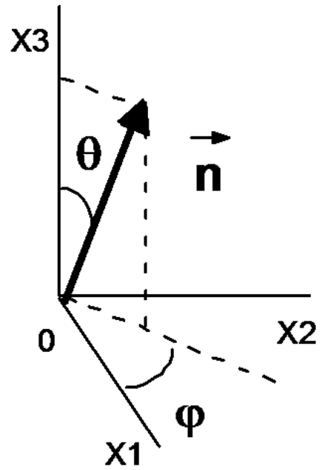
$$K_{eff}(\vec{n}) = n_i K_{ij} n_j$$

$$\rho(\vec{n}) = \frac{1}{\sqrt{K_{eff}(\vec{n})}}$$

Example: calculation of effective dielectric constant

Material: rutile (TiO_2), tetragonal, 4/mmm $\qquad K_{\parallel} = 173 \text{ et } K_{\perp} = 89$

$$K_{eff} = n_i K_{ij} n_j \text{ ou } K_{eff} = \vec{n}\,\underline{K}\,\vec{n}$$



$$n_j = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}$$

$$K_{eff} = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix} * \begin{pmatrix} K_{\perp} & 0 & 0 \\ 0 & K_{\perp} & 0 \\ 0 & 0 & K_{\parallel} \end{pmatrix} * \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix} = K_{\parallel}\cos^2\theta + K_{\perp}\sin^2\theta$$

For example, for θ=45°: $\qquad K_{eff} = \dfrac{K_{\perp} + K_{\parallel}}{2} = \dfrac{179+89}{2} = 131$

Polycrystalline dielectrics with randomly oriented grains

In the principal axes

$$K_{eff}(\vec{n}) = n_1^2 K^{(1)} + n_2^2 K^{(2)} + n_3^2 K^{(3)}$$

Randomly oriented grains:

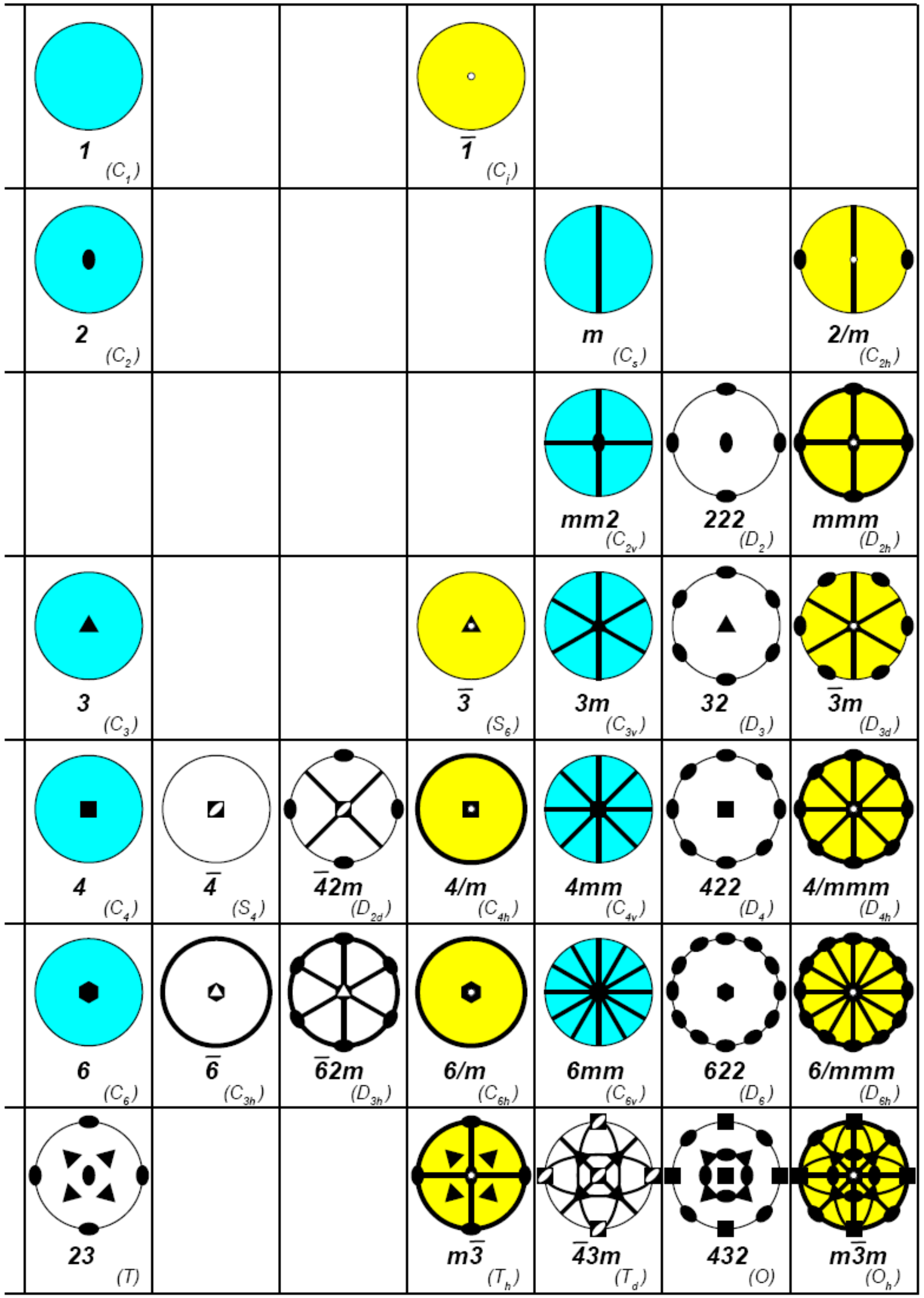
$$\langle K \rangle = 1/3(K_{11} + K_{22} + K_{33})$$

The polycrystalline dielectric constant is simply the numerical average of the principal dielectric constants

3 types of dielectric anisotropy

Tensor	Ellipsoid	anisotropy
$K^{(1)} = K^{(2)} = K^{(3)}$	Sphere	isotropic
$K^{(1)} = K^{(2)} \neq K^{(3)}$	Rotational ellipsoid	uniaxial
$K^{(1)} \neq K^{(2)} \neq K^{(3)} \neq K^{(1)}$	General ellipsoid	biaxial (general)

Symmetry of the dielectric response (3 types)



$$mmm$$

$$\begin{pmatrix} K_{11} & 0 & 0 \\ & K_{22} & 0 \\ & & K_{33} \end{pmatrix}$$

∞ $\quad$ ∞m

$\infty 2$ $\quad$ ∞ / m

∞ / mm

$$\infty / mm$$

$$\begin{pmatrix} K_1 & 0 & 0 \\ & K_1 & 0 \\ & & K_3 \end{pmatrix}$$

$\infty\infty m$ $\quad$ $\infty\infty$

$$\begin{pmatrix} K & 0 & 0 \\ & K & 0 \\ & & K \end{pmatrix}$$

$$\infty\infty m$$

Link: material symmetry - tensor structure in conventional axes

39 groups of macroscopic symmetry

↓

5 structures of K-tensor

$$\begin{pmatrix} K_{11} & K_{12} & 0 \\ & K_{22} & 0 \\ & & K_{33} \end{pmatrix} \quad \begin{pmatrix} K_{11} & K_{12} & K_{13} \\ & K_{22} & K_{23} \\ & & K_{33} \end{pmatrix}$$

5

$$\begin{pmatrix} K_{11} & 0 & 0 \\ & K_{22} & 0 \\ & & K_{33} \end{pmatrix}$$

$$\begin{pmatrix} K & 0 & 0 \\ & K & 0 \\ & & K \end{pmatrix} \quad \begin{pmatrix} K_{1} & 0 & 0 \\ & K_{1} & 0 \\ & & K_{3} \end{pmatrix}$$

Results of application of Neumann principle

Link:
material symmetry –property symmetry

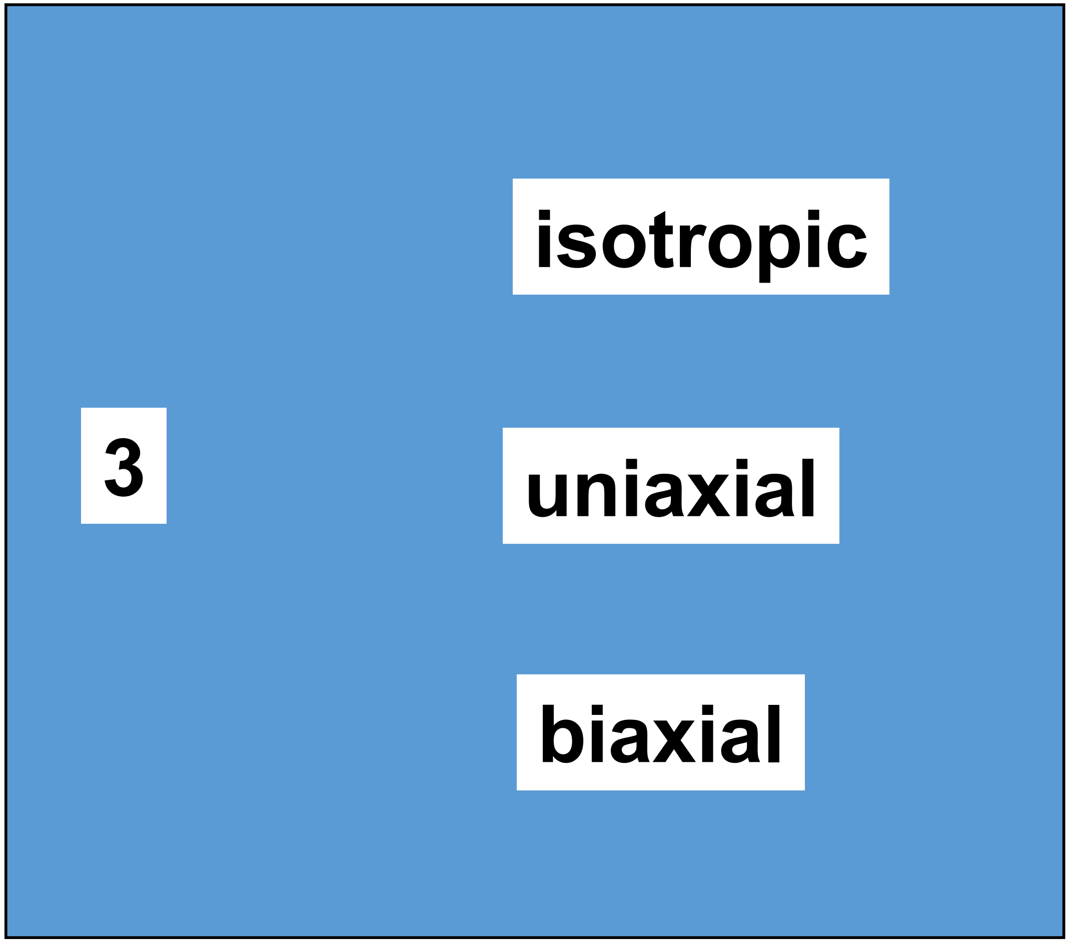
39 groups of macroscopic symmetry

↓

5 structures of K-tensor

↓

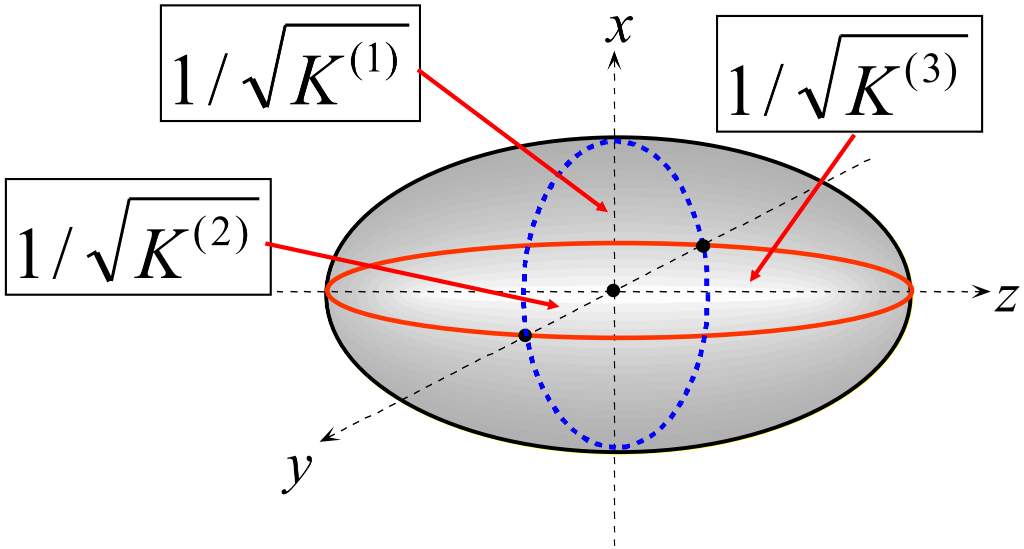
3 types of property symmetry



Result of anisotropy of dielectric response

Symmetry of dielectric response in terms of representation quadrics

In principal axes of the tensor

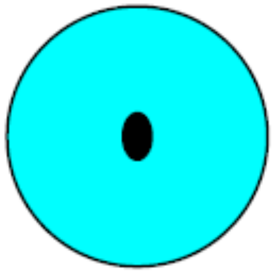


$$\begin{pmatrix} K^{(1)} & 0 & 0 \\ & K^{(2)} & 0 \\ & & K^{(3)} \end{pmatrix}$$

Symmetry of ellipsoid **=** **Symmetry of tensor** **=** **Symmetry of property**

Obvious additional symmetry elements of the property

material

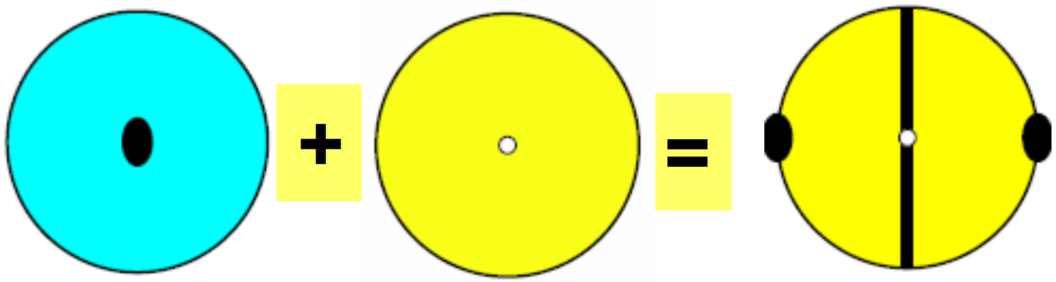


2

$$\begin{pmatrix} K_{11} & 0 & K_{13} \\ & K_{22} & 0 \\ & & K_{33} \end{pmatrix}$$

ellipsoid

Any ellipsoid is invariant with respect to inversion!

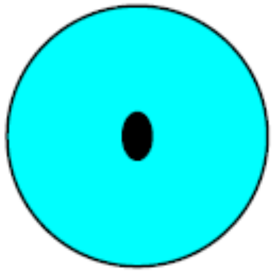


2 $\bar{1}$ **2/m**

property

Hidden symmetry elements of property

material



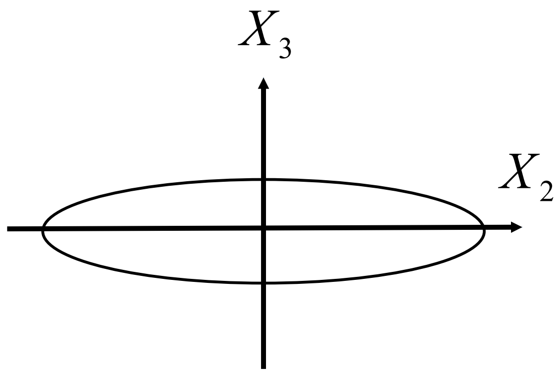
2

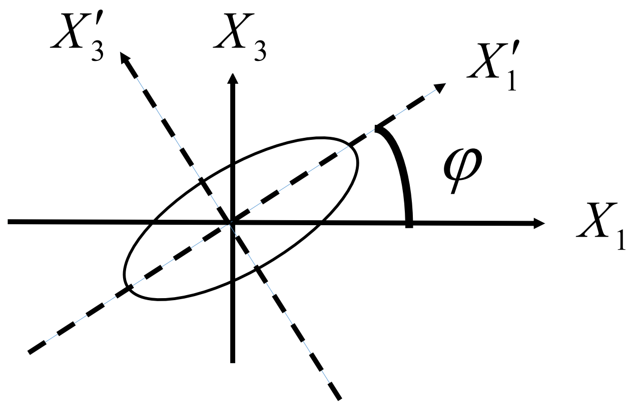
$$\begin{pmatrix} K_{11} & 0 & K_{13} \\ & K_{22} & 0 \\ & & K_{33} \end{pmatrix}$$

$$K_{11}X_1^2 + K_{33}X_3^2 + 2K_{13}X_1X_3 + K_{22}X_2^2 = 1$$

$$\begin{pmatrix} K'_{11} & 0 & 0 \\ & K_{22} & 0 \\ & & K'_{33} \end{pmatrix}$$

$$K'_{11}X_1^2 + K'_{33}X_3^2 + K_{22}X_2^2 = 1$$

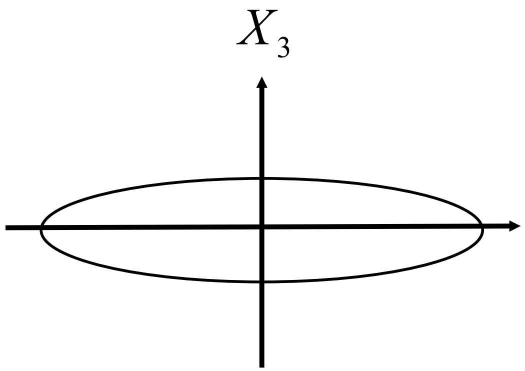




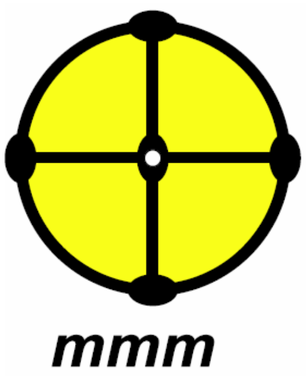
$$\tan\varphi = \frac{K_{13}}{K_{11} - K'_{11}}$$

Hidden symmetry elements of property

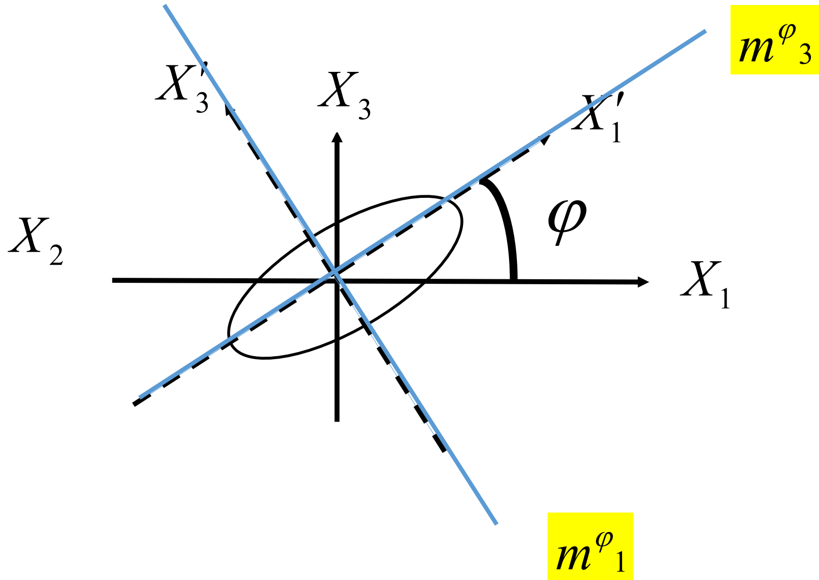
High symmetry (orthorhombic or higher)



Symmetry of ellipsoid Conventional axes of the material



Low symmetry



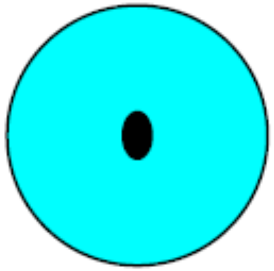
The orientations of the hidden symmetry elements depend on the property

For instance, for dielectric response and conductivity the orientation of principle axes is not same

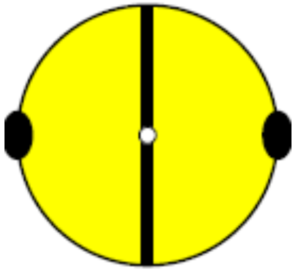
Low symmetry: orientation of hidden symmetry elements is different for different properties

Two different properties:

material



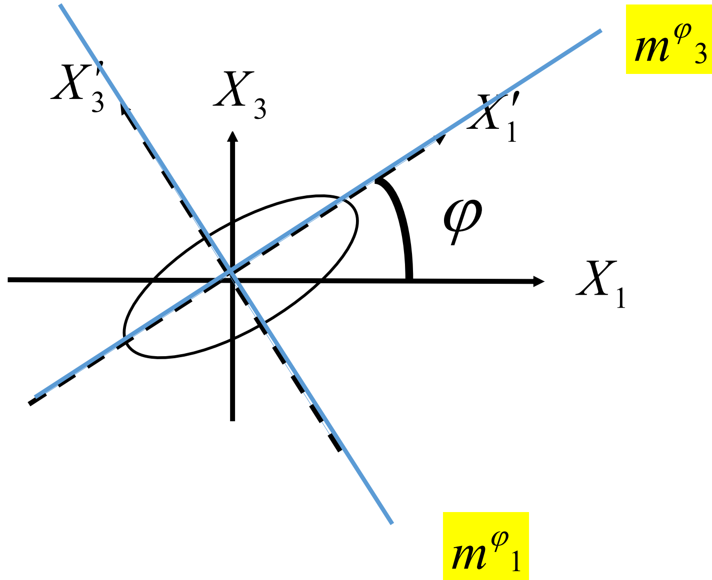
2



2/m

$$\begin{pmatrix} K_{11} & 0 & K_{13} \\ & K_{22} & 0 \\ & & K_{33} \end{pmatrix}$$

$$\begin{pmatrix} \alpha_{11} & 0 & \alpha_{13} \\ & \alpha_{22} & 0 \\ & & \alpha_{33} \end{pmatrix}$$



$$\tan\varphi_K = \frac{K_{13}}{K_{11} - K'_{11}}$$

$$\tan\varphi_\alpha = \frac{\alpha_{13}}{\alpha_{11} - \alpha'_{11}}$$

$$\varphi_\alpha \neq \varphi_K$$

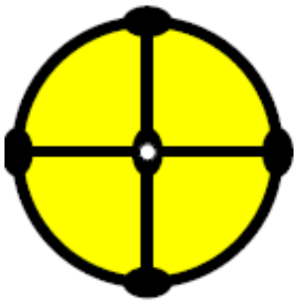
Diagonal form is not available for two properties at once !

Comparison with *mmm* materials Symmetry

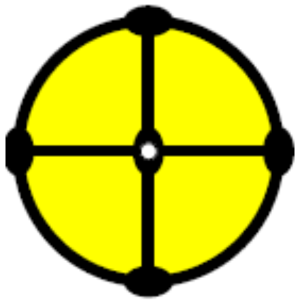
High symmetry (orthorhombic or higher): diagonal form is available for two properties at once !

All properties controlled by such type of tensor

material



mmm

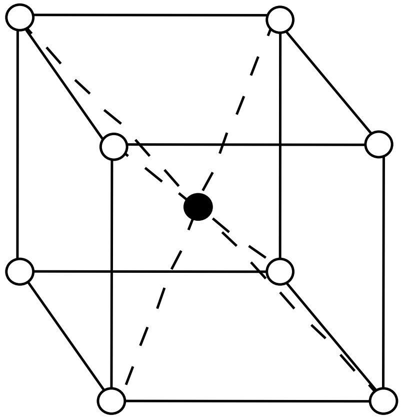


mmm

$$\begin{pmatrix} K_{11} & 0 & 0 \\ & K_{22} & 0 \\ & & K_{33} \end{pmatrix}$$

$$\begin{pmatrix} \alpha_{11} & 0 & 0 \\ & \alpha_{22} & 0 \\ & & \alpha_{33} \end{pmatrix}$$

Dielectric response: examples of materials

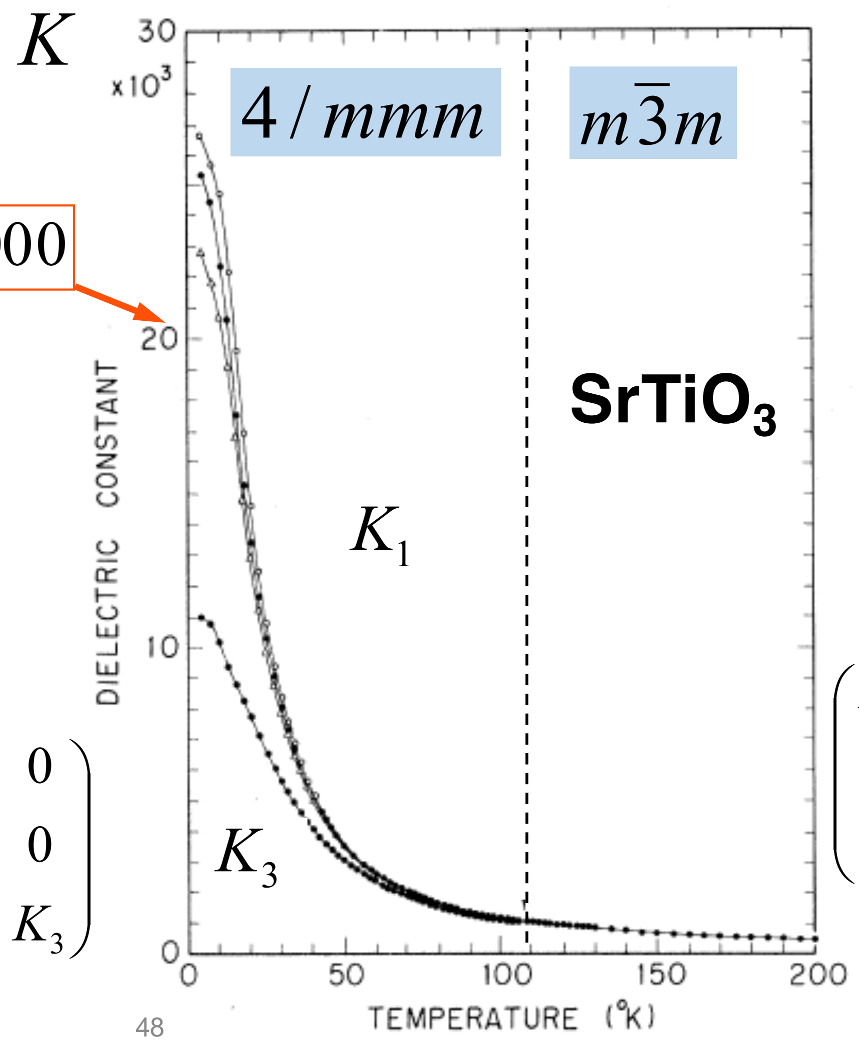


$m\bar{3}m$ **CsCl**

$$\begin{pmatrix} K & 0 & 0 \\ & K & 0 \\ & & K \end{pmatrix}$$

$$K = 6.3$$

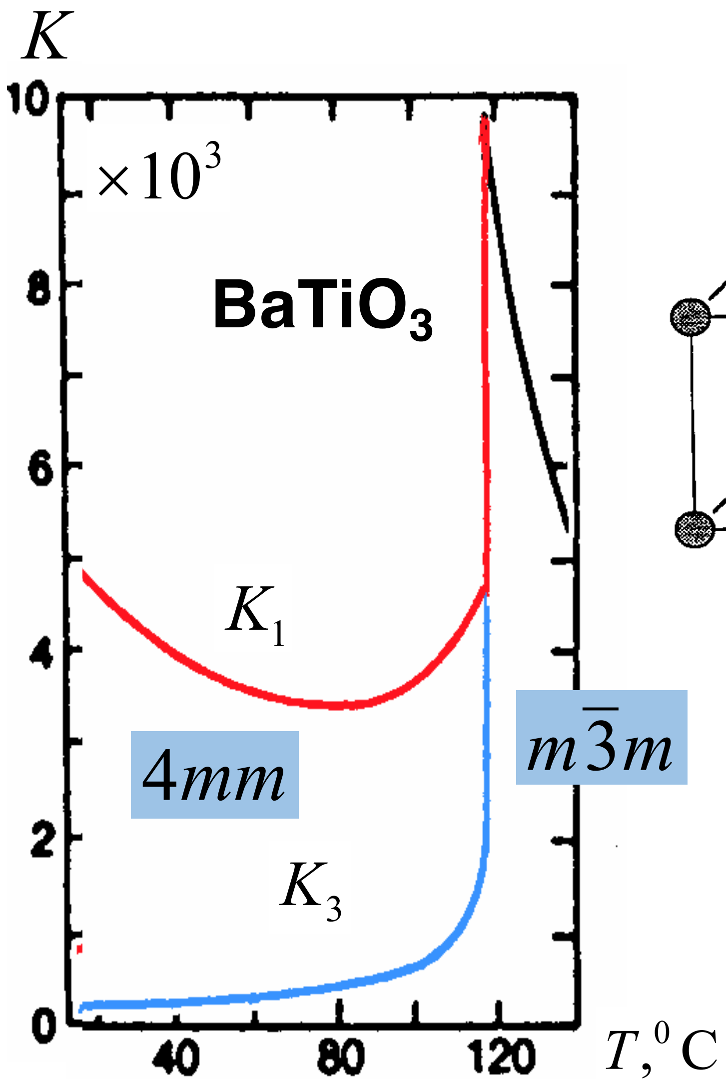
20 000

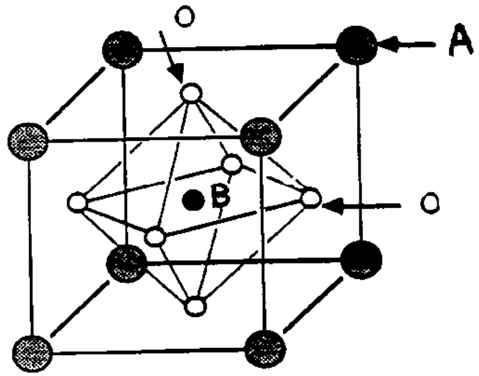


$$\begin{pmatrix} K_1 & 0 & 0 \\ & K_1 & 0 \\ & & K_3 \end{pmatrix}$$

$$\begin{pmatrix} K & 0 & 0 \\ & K & 0 \\ & & K \end{pmatrix}$$

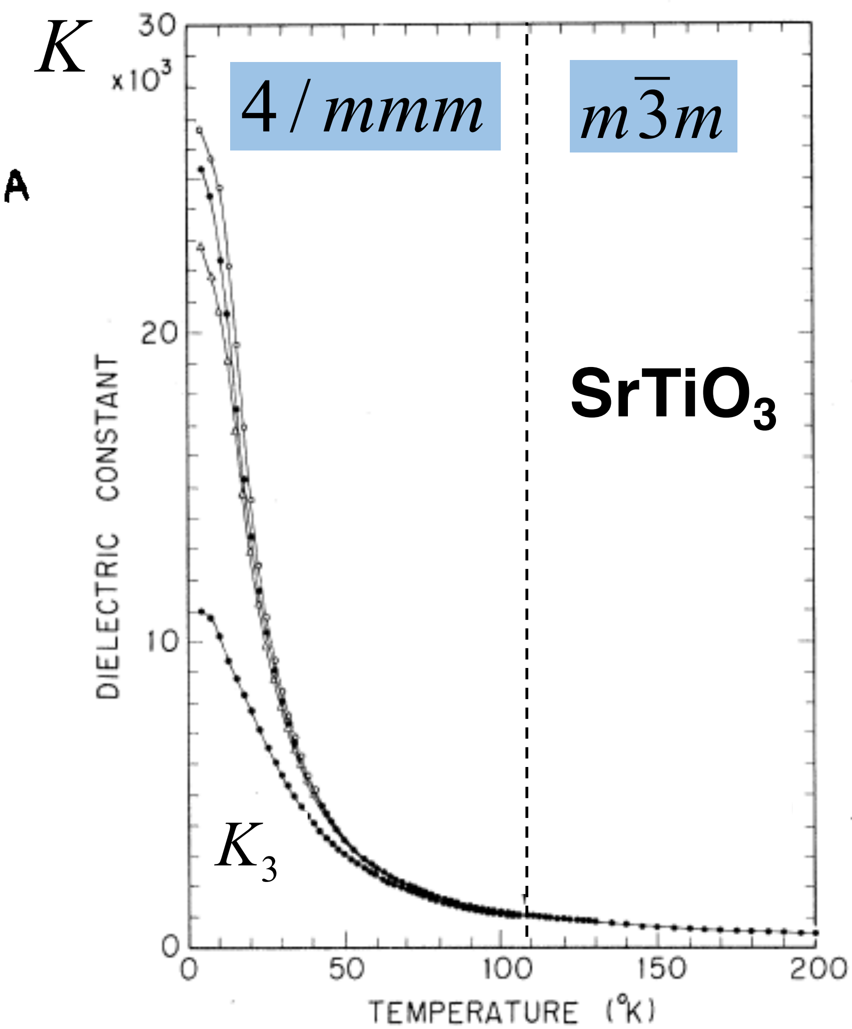
Dielectric response:
examples of materials-perovskites





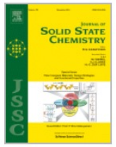
$A = Ba, Sr$

$B = Ti$



Definition of polarization: modern theory

Journal of Solid State Chemistry
Volume 195, November 2012, Pages 2-10



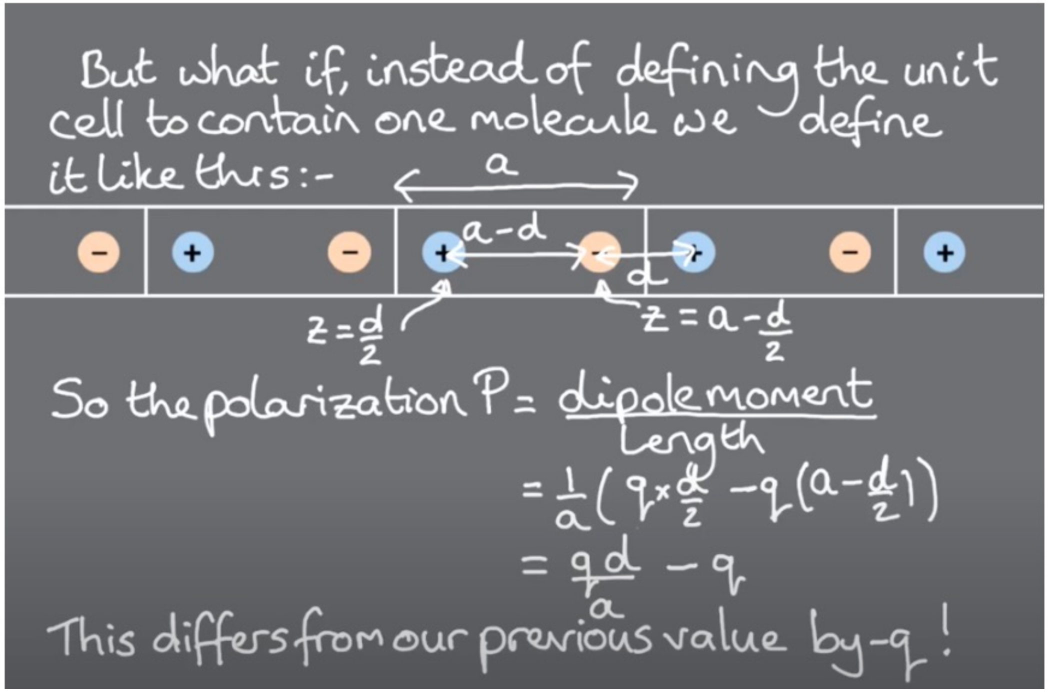
A beginner's guide to the modern theory of polarization

Nicola A. Spaldin

https://doi.org/10.1016/j.jssc.2012.05.010

(optional reading)

Youtube resources: lecture of Prof. Nicola Spaldin



https://www.youtube.com/watch?v=UtLKjTPEKTk

- Accurate definition of polarization is not that simple

- For practical applications a change of polarization vs external stimuli (e.g. changing electric field) is important

Essential – application Neumann principle to dielectric response, part I

1. The symmetry of a material can be translated into that of a property by the Neumann principle.

2. The symmetry of a property is controlled by the internal symmetry of the tensor and the symmetry of the material. The symmetry of a property = the symmetry of a tensor describing the property.

3. The symmetry of property is not lower (can be higher!) than that of the material.

4. Symmetry-based analysis performed here for dielectric response can be extended to other phenomena described by symmetric second-rank tensors