ELECTRONICS DEVICES AND MATERIALS

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SYLLABUS

- Introduction to materials structure and dielectric physics
- Ferroelectricity involved in structural phase transitions
- Material design of dielectrics and introduction to metamaterials
- Ferroelectric devices

TODAY'S TOPICS

1. What is Dielectric?

2. Dielectricity of Materials and Dielectric Dispersion

- Electric Polarizations in Solid State Materials and Dielectric Constant
- Electric Dipoles and Polarizability
- Dielectric Dispersion (Relaxation &Resonance type)

3. Crystal Structures and Their Symmetry

- Crystal System and The Bravais lattices
- Symmetry Operations and Point Goups
- Crystal symmetry and Polar Crystals

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WHAT IS DIELECTRIC?

A ‘dielectric’ is a good electric insulator so as to minimize any DC leakage current through a dielectric material.

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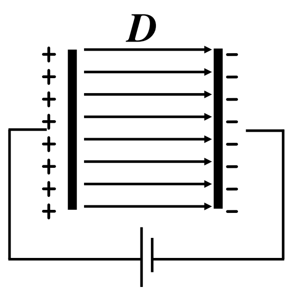
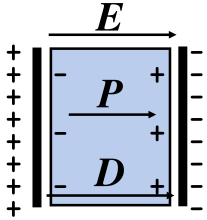
POLARIZATION OF DIELECTRIC

Vacuum



Dielectric



Electric susceptibility: χ

polarization density: ***P***

$$\boldsymbol{D}=\varepsilon_0 \boldsymbol{E} + \boldsymbol{P}$$

$$\boldsymbol{P}=\varepsilon_0 \chi \boldsymbol{E}$$

$$\boldsymbol{D}=\varepsilon_0 (1+\chi) \boldsymbol{E}$$

$$=\varepsilon_r \varepsilon_0 \boldsymbol{E}$$

relative permittivity: ε_r

Relationship of electric displacement field, ***D*** and electric field, ***E***

$$\boldsymbol{D}=\varepsilon_0 \boldsymbol{E}$$

COMPLEX PERMITTIVITY (COMPLEX ELECTRIC CONSTANT)

Erectric Field E
⇒alternating current(AC) Field

$$E=E_0 e^{j\omega t}$$

electric displacement field, **D**

$$D=D_0 e^{j\omega t-\delta}$$

δ : measurable phase difference emerging between **D** and **E**

$$D=\varepsilon_0 \varepsilon^* E$$

Complex permittivity: ε^*

$$\varepsilon^* = \varepsilon' - \varepsilon''$$

$$\varepsilon' = \frac{D_0}{\varepsilon_0 E_0} \cos\delta$$

$$\varepsilon'' = \frac{D_0}{\varepsilon_0 E_0} \sin\delta$$

$$\tan\delta = \frac{\varepsilon''}{\varepsilon'}$$

W is a energy stored in dielectric.

$$W=\frac{1}{2}\omega \varepsilon'' \varepsilon_0 E_0^2$$

$$=\frac{1}{2}\omega \varepsilon' \varepsilon_0 E_0 \tan\delta^2$$

ε'' and $\tan\delta$ are related to the dissipation (or loss) of energy within the medium.

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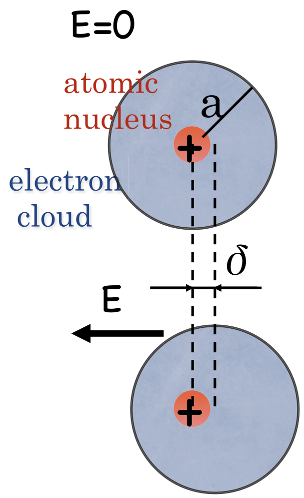
ORIGINS OF POLARIZATION ~ ELECTRONIC POLARIZATION ~



Electron electric dipole moment : μ_e

$$\mu_e = \alpha_e E$$

Electron polarizability : α_e

$$\alpha_e = 4\pi\varepsilon_0 a^3$$

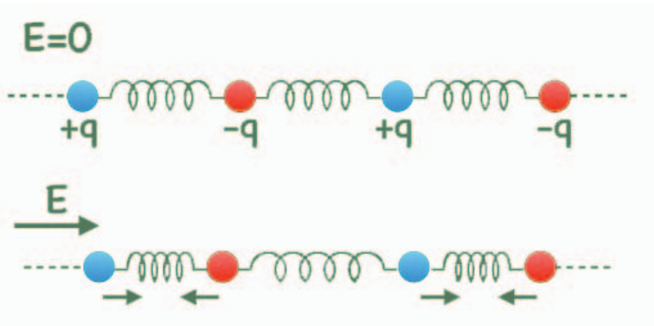
⇒proportional to atomic volume

Polarizability of mono-atomic ion (10^{-24} cm^3)

Li^{+1}	Be^{+2}	B^{+3}	C^{+4}	O^{-2}	F^{-1}	Ne
0.029	0.008	0.003	0.0013	3.88	1.04	0.390
Na^{+1}	Mg^{+2}	Al^{+3}	Si^{+4}	S^{-2}	Cl^{-1}	Ar
0.179	0.094	0.052	0.0165	10.2	3.66	1.62
K^{+1}	Ca^{+2}	Sc^{+3}	Ti^{+4}	Se^{-2}	Br^{-1}	Kr
0.83	0.47	0.286	0.189	10.5	4.77	2.46
Rb^{+1}	Sr^{+2}	Y^{+3}	Zr^{+4}	Te^{-2}	I^{-1}	Xe
1.40	0.86	0.55	0.37	14.0	7.10	3.99
Cs^{+1}	Ba^{+2}	La^{+3}				
2.42	1.55	1.04				

Paulng's values

ORIGINS OF POLARIZATION ~ IONIC POLARIZATION (ATOMIC POL.) ~



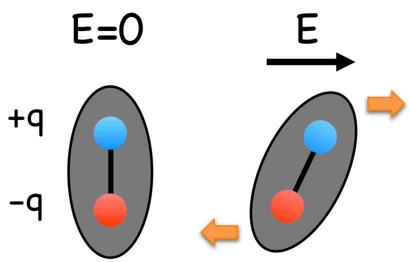
Ionic electric dipole moment : μ_i

$$\mu_i = \alpha_i E$$

Ionic or Atom polarizability : α_i

ORIGINS OF POLARIZATION ~ DIPOLAR POLARIZATION (DIPOLE RELAXATION) ~

Many molecules have permanent dipole moments μ due to non-uniform distributions of positive and negative charges on the various atoms.



The orientation is induced by electric field.

Behavior of Dipole moment in electric field is given by Classical Statics (Boltzmann distribution).

$$\alpha_p = \frac{\mu}{3kT}$$

⇒Polarization decrease with increasing temperature due to atomic vibrations.

ORIGINS OF POLARIZATION

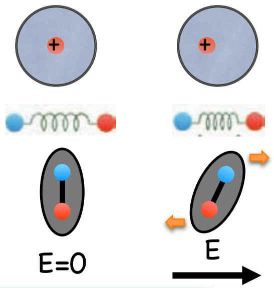
- Electronic Polarization, α_e
- Ionic Polarization, α_i

- Ionic Crystals, NaCl

- Dipolar Polarization, α_o

- Polar Molecules, HCl

- Space Charge Polarization, α_s



The total polarizability of the dielectric:

$$\alpha = \alpha_e + \alpha_i + \alpha_o + (\alpha_s)$$

$$\alpha = \alpha_e + \alpha_i + \frac{\mu}{3kT}$$

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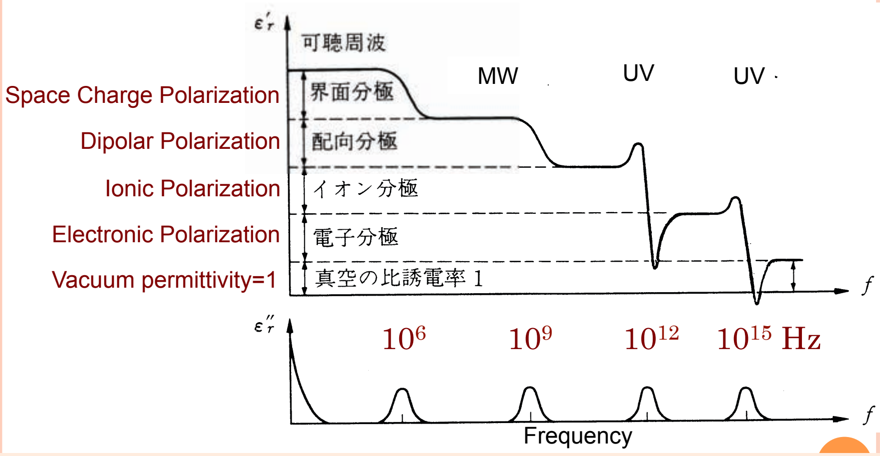
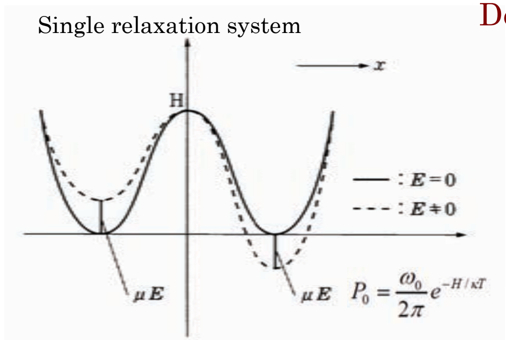
DIELECTRIC DISPERSION ~ DIELECTRIC SPECTROSCOPY ~



Dielectric dispersion is the dependence of the permittivity of a dielectric material on the frequency of an applied electric field.

RELAXATION TYPE DISPERSION



The energy barrier for the relaxation type dielectric dispersion.

Debye relaxation equations

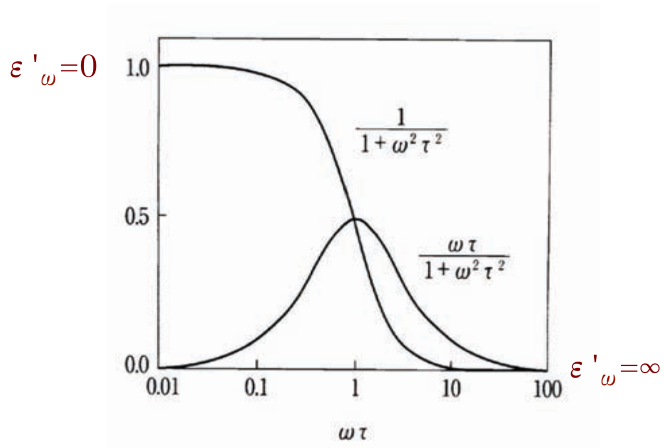
$$\varepsilon^*(\omega) = \varepsilon(\infty) + \frac{\varepsilon(0) - \varepsilon(\infty)}{1 + i\omega\tau}$$

$$\varepsilon'(\omega) = \varepsilon(\omega) + \frac{\varepsilon(0) - \varepsilon(\infty)}{1 + \omega^2\tau^2}$$

$$\varepsilon''(\omega) = \frac{\{\varepsilon(0) - \varepsilon(\infty)\}\omega\tau}{1 + \omega^2\tau^2}$$

τ : relaxation time

RELAXATION TYPE DISPERSION



Relaxation spectra of relative dielectric constant, conductivity, and loss factor for a simple relaxation process with a single relaxation.

RESONANCE TYPE DISPERSION

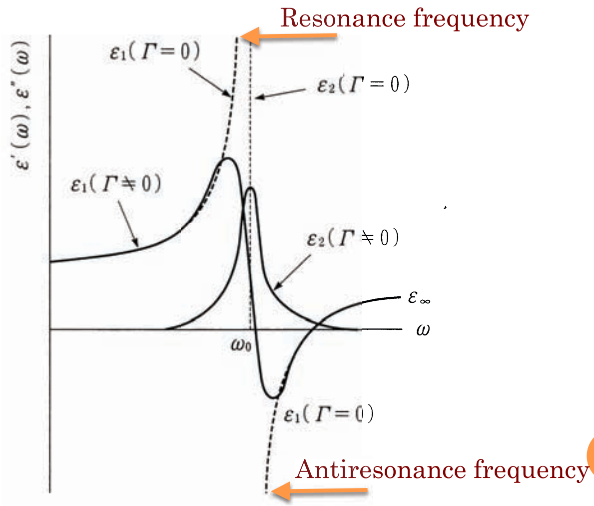
Resonance effects:
the rotations or vibrations of atoms, ions, or electrons.

$$\varepsilon^*(\omega) = \varepsilon(\infty) + \frac{\{\varepsilon(0)-\varepsilon(\infty)\}\omega_0^{\ 2}}{\omega_0^{\ 2} - \omega^2 + i\Gamma\omega^2}$$

$$\varepsilon'(\omega) = \varepsilon(\infty) + \frac{\{\varepsilon(0)-\varepsilon(\infty)\}\omega_0^{\ 2}(\omega_0^{\ 2}-\omega^2)}{(\omega_0^{\ 2}-\omega^2)^2 + \Gamma^2\omega^2}$$

$$\varepsilon''(\omega) = \frac{\{\varepsilon(0)-\varepsilon(\infty)\}\omega_0^{\ 2}\Gamma\omega}{(\omega_0^{\ 2}-\omega^2)^2 + \Gamma^2\omega^2}$$

RESONANCE TYPE DISPERSION



Frequency response near resonance of a dielectrics.

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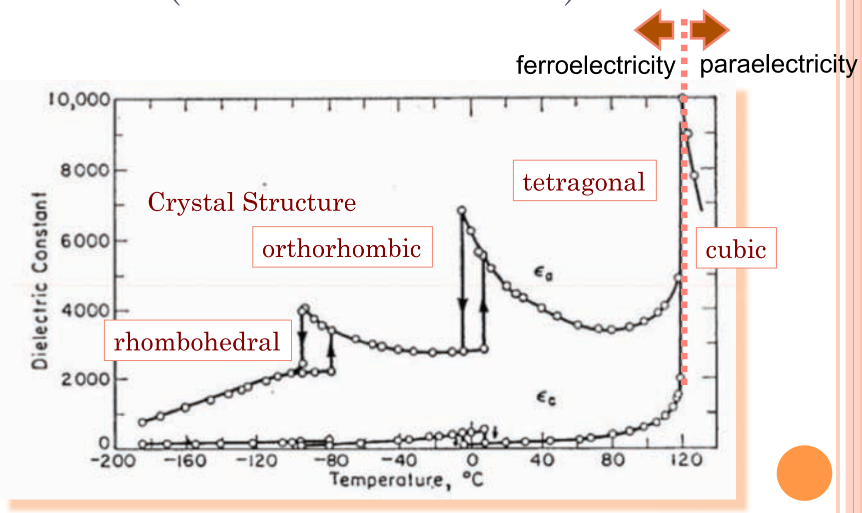
BATIO3 (BARIUM TITANATE)



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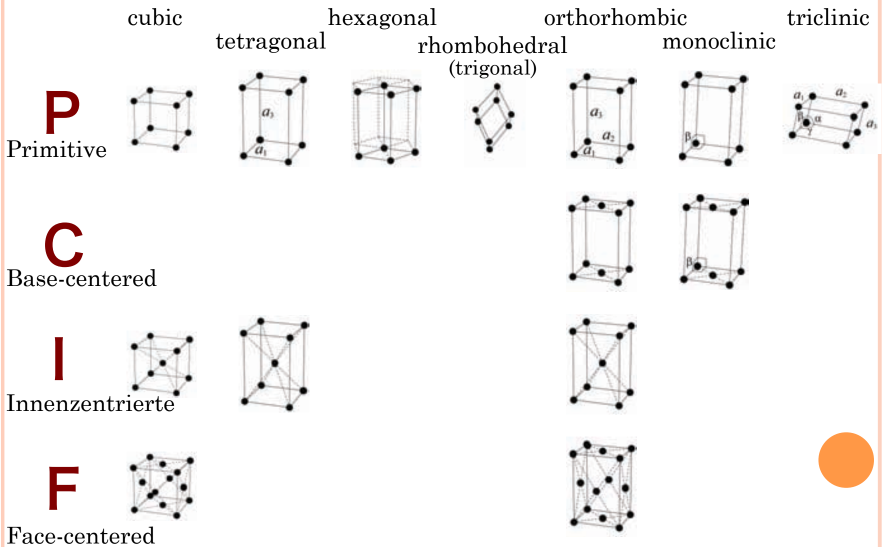
THE 7 CRYSTAL SYSTEMS

Cubic	$\alpha=\beta=\gamma=90^\circ$	a=b=c
Tetragonal	$\alpha=\beta=\gamma=90^\circ$	a=b≠c
Hexagonal	$\alpha=\beta=90^\circ;\gamma=120^\circ$	a=b; c
Rhombohedral	$\alpha=\beta=\gamma\neq90^\circ$	a=b=c
Orthorhombic	$\alpha=\beta=\gamma=90^\circ$	a<b<c
Monoclinc	$\alpha=\gamma=90^\circ,\ \beta\neq90^\circ$	c≤a,b
Triclinic	$\alpha\neq90^\circ,\ \beta\neq90^\circ,\ \gamma\neq90^\circ$	c≤a≤b

THE 14 BRAVAIS LATTICE



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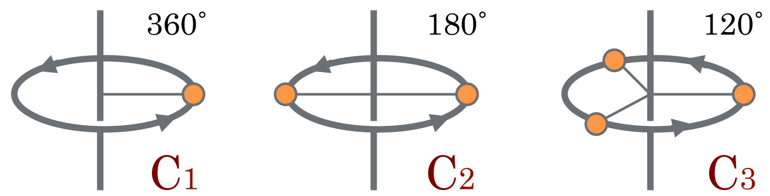
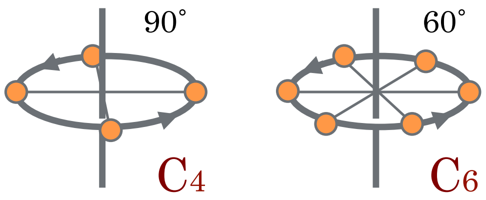
SYMMETRY OPERATIONS

Rotation	回転(5種類)
Reflection	鏡映(反射)
Inversion	反転
Rotatory inversion	回反
Rotatory reflection	回映

ROTATION SYMMETRY





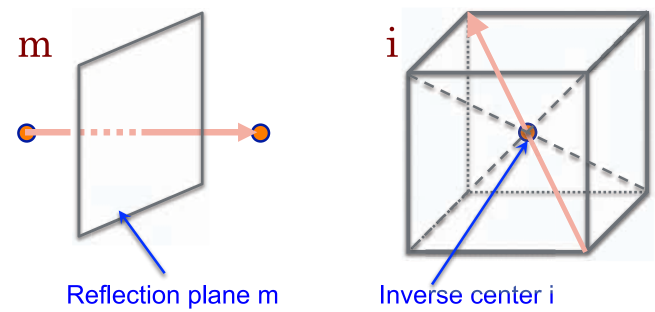
Symbol: C_n

n=1,2,3,4,6

Rotation by 360˚/n or 2π/n about a rotation axis

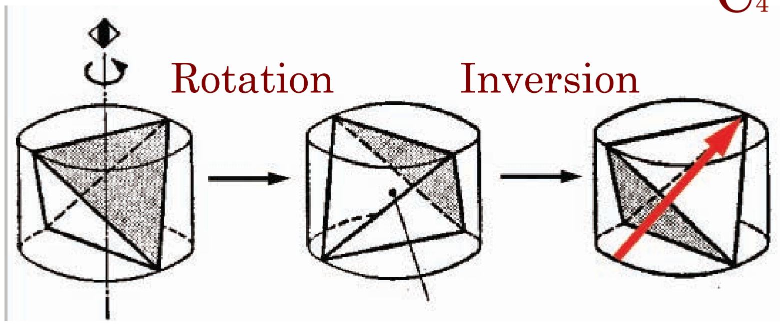
REFLECTION AND INVERSION SYMMETRY

Reflection: m (or σ) Inversion: i (or I)

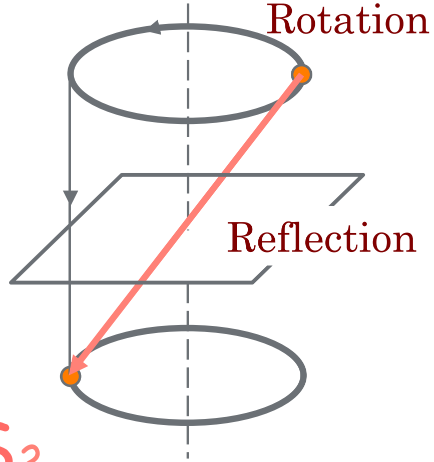


ROTATORY INVERSION SYMMETRY

$\overline{C}_4$



ROTATORY REFLECTION SYMMETRY



$S_1 = m$
$S_2 = i$
$S_3 = C_3+m$
$S_6 = C_3+i$

SYMMETRY ELEMENT IN CRYSTALLOGRAPHY

Identity transformation: **E** = C_1

- Rotation axis **C_1, C_2, C_3, C_4, C_6**
- Rotation Inversion axis **$\overline{C}_3$, $\overline{C}_4$, $\overline{C}_6$**
- Rotation Reflection axis **S_3, S_4, S_6**
- Reflection plane **m**
- Inversion center **i**

There are **the 13 symmetry elements** in crystals.

HERMANN-MAUGUIN NOTATION ~ INTERNATIONAL SYMBOL ~

	Schoenflies Symbols	International Symbols
Rotation axis	C_1, C_2, C_3, C_4, C_6	1, 2, 3, 4, 6
Rotation Inversion axis	$\overline{C}_3$, $\overline{C}_4$, $\overline{C}_6$	$\overline{3}$, $\overline{4}$, $\overline{6}$
Rotation Reflection axis	S_3, S_4, S_6	3/m, 4/m, 6/m
Reflection plane	m	m
Inversion center	i	$\overline{1}$

POINT GROUPS

	Schönflies Notation	Hermann -Maugum
Cubic	O_h	m3m
	O	432
	T_d	$\bar{4}3m$
	T_h	m3
	T	23

O (octahedron) :
The group has the symmetry of an octahedron (or cube), with (O_h) or without (O) improper operations (those that change handedness).

T (tetrahedron)
The group has the symmetry of a tetrahedron. T_d includes improper operations, T excludes improper operations, and T_h is T with the addition of an inversion.

POINT GROUPS

	Schönflies Notation	Hermann -Maugum
Tetragonal	D_{4h}	4/mmm
	D_4	422
	D_{2d}	$\bar{4}2m$
	C_{4v}	4mm
	C_{4h}	4/m
	S_4	$\bar{4}$
	C_4	4

S_n (Spiegel):
The group that contains only an n-fold rotation-reflection axis.

D_n (dihedral):
The group has an n-fold rotation axis plus a twofold axis perpendicular to that axis. D_{nh} has, in addition, a mirror plane perpendicular to the n-fold axis. D_{nv} has, in addition to the elements of D_n, mirror planes parallel to the n-fold axis.

C_n (cyclic):
The group has an n-fold rotation axis. C_{nh} is C_n with the addition of a mirror (reflection) plane perpendicular to the axis of rotation. Cnv is C_n with the addition of a mirror plane parallel to the axis of rotation.

POINT GROUPS

	Schönflies Notation	Hermann -Maugum
Hexagonal	D_{6h}	6/mmm
	D_6	622
	D_{3h}	6m2
	C_{6v}	6mm
	C_{6h}	6/m
	C_{3h}	$\bar{6}$
	C_6	6

Subscripts (h, v, d, i)

h: Horizontal reflection plane - passing through the origin and perpendicular to the axis with the 'highest' symmetry.

v: Vertical reflection plane - passing through the origin and the axis with the 'highest' symmetry.

d: Diagonal or dihedral reflection in a plane through the origin and the axis with the 'highest' symmetry, but also bisecting the angle between the twofold axes perpendicular to the symmetry axis.

i: inverse

POINT GROUPS

	Schönflies Notation	Hermann -Maugum
Rhombohedral	D_{3d}	$\bar{3}m$
	D_3	32
	C_{3v}	3m
	C_{3i}	$\bar{3}$
	C_3	3
Orthorhombic	D_{2h}	mmm
	D_2	222
	D_{2v}	mm2

POINT GROUPS

	Schönflies Notation	Hermann -Maugum
Monoclinic	C_{2h}	2/m
	C_S	m
	C_2	2
Triclinic	C_i	1
	C_1	$\bar{1}$

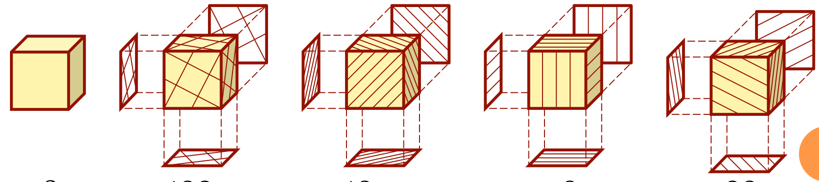
There are the 32 point group types.

Compound symmetry: screw axis and glide plane symmetry operations

The 230 unique space groups describing all possible crystal symmetries

POINT GROUPS OF CUBIC SYSTEM

	Schönflies Notation	Hermann -Maugum
Cubic	O_h	m3m
	O	432
	T_d	$4\bar{3}m$
	T_h	m3
	T	23



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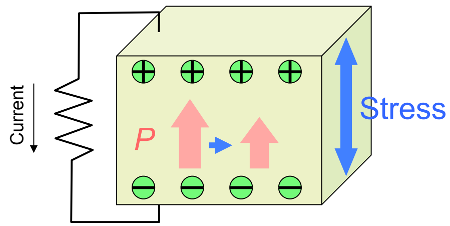
PIEZOELECTRICITY AND CENTER OF SYMMETRY

Piezoelectricity : the ability of some materials to generate an electric potential in response to applied mechanical stress



Notice : **Piezoelecticity** is a linear effect, unlike **electrostriction**, which is a quadratic effect. In addition, **electrostriction** cannot be reversed, unlike **piezoelectricity**: deformation will not induce an electric field.

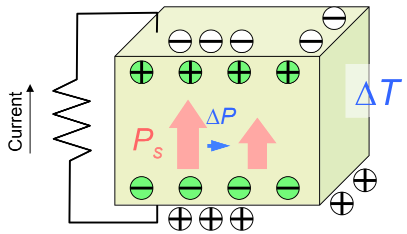
The formation of a separation of electric charge across the crystal lattice

20 piezoelectric point-groups lack a center of symmetry.

(the 21st is the cubic class 432)

PYOELECTRICITY AND SPONTANEOUS POLARIZATION

Pyroelectricity:
Spontaneous polarization is temperature dependent



$$\Delta P_i = p_i \, \Delta T$$

pyroelectric coefficient

Pyroelectric Crystal shows **spontaneous polarization**, having a dipole in their unit cell.

What is a origin of spontaneous polarization in crystal structure?

POLAR VECTOR

In Descartes mathematics, An example of an improper rotation is a mirror reflection. That is, these vectors are defined in such a way that, if all of space were flipped around through a mirror (or otherwise subjected to an improper rotation), that vector would flip around in exactly the same way.

As a particular case where the symmetry group is important, all of the below physical examples are vectors which "transform like the coordinates" under both proper and improper rotations. Vectors with this property are sometimes called **true vectors.**

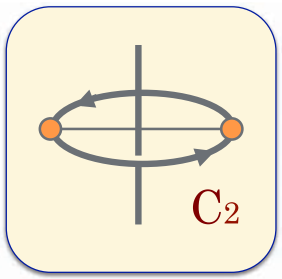
Physical examples:
displacement, velocity, electric field, momentum, force, acceleration.

Axial vector (pseudovectors) :a quantity that transforms like a vector under a proper rotation, but gains an additional sign flip under an improper rotation (a transformation that can be expressed as an inversion followed by a proper rotation).

Physical examples:
the magnetic field, torque, vorticity, the angular momentum.

POLAR VECTOR AND SYMMETRY OPERATION
~ PYROELECTRICITY AND SPONTANEOUS POLARIZATION ~

2-fold symmetry C2 : (x, y, z) ⇒ (-x, -y, z)



$$\begin{bmatrix} P'_1 \\ P'_2 \\ P'_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} P_1 \\ P_2 \\ P_3 \end{bmatrix} = \begin{bmatrix} -P_1 \\ -P_2 \\ P_3 \end{bmatrix}$$

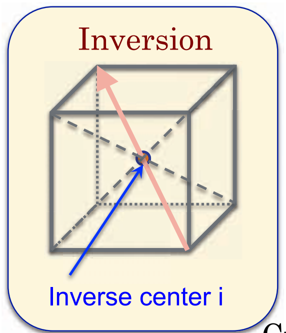
von Neumann's theorem : $P'_i = P_i$

$$\boldsymbol{P_1 = P_2 = 0,\ P_3 \neq 0}$$

Component of polar vector; **(0, 0, z)**
⇒ Occurrence of Spontaneous polarization

POLAR VECTOR AND SYMMETRY OPERATION
~ PYROELECTRICITY AND SPONTANEOUS POLARIZATION ~

Inverse symmetry **i** : (x, y, z) ⇒ (-x, -y, -z)



$$\begin{bmatrix} P'_1 \\ P'_2 \\ P'_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} P_1 \\ P_2 \\ P_3 \end{bmatrix} = \begin{bmatrix} -P_1 \\ -P_2 \\ -P_3 \end{bmatrix}$$

von Neumann's theorem : $P'_i = P_i$

$$\boldsymbol{P_1 = P_2 = P_3 = 0}$$

Crystals including inverse symmetry do not have spontaneous polarization.

POLAR VECTOR AND SYMMETRY OPERATION
~ 10 POINT GROUPS IS POLAR ~

Point Group	Component of polar vector
2, 2m, 3, 3m, 4 4m, 6, 6m	0, 0, p_3
m	p_1, p_2, 0
1	p_1, p_2, p_3

Component of spontaneous polarization
Component of pyroelectric coefficient

PIEZOELECTRICITY, PYROELECTRICITY AND FERROELECTRICITY

Piezoelectricity

20 point groups lacking in a center of symmetry

Pyroelectricity

10 point groups including polar vectors
(having spontaneous polarization)

Ferroelectricity

The direction of spontaneous polarization can be switched between equivalent states by the application of an external electric field.

POINT GROUPS

	Schönflies Notation	Hermann -Maugum	Inversion Center	Polar Vector
Cubic	O_h	m3m	√	0
	O	432	-	0
	T_d	$\bar{4}3m$	-	0
	T_h	m3	√	0
	T	23	-	0

POINT GROUPS

	Schönflies Notation	Hermann -Maugum	Inversion Center	Polar Vector
Tetragonal	D_{4h}	4/mmm	√	0
	D_4	422	-	0
	D_{2d}	$\bar{4}2m$	-	0
	C_{4v}	4mm	-	(0, 0, z)
	C_{4h}	4/m	√	0
	S_4	$\bar{4}$	-	0
	C_4	4	-	(0, 0, z)

POINT GROUPS

	Schönflies Notation	Hermann -Maugum	Inversion Center	Polar Vector
Hexagonal	D_{6h}	6/mmm	√	0
	D_6	622	-	0
	D_{3h}	6m2	-	0
	C_{6v}	6mm	-	(0, 0, z)
	C_{6h}	6/m	√	0
	C_{3h}	$\bar{6}$	-	0
	C_6	6	-	(0, 0, z)

POINT GROUPS

	Schönflies Notation	Hermann -Maugum	Inversion Center	Polar Vector
Rhombohedral	D_{3d}	$\bar{3}$m	√	0
	D_3	32	-	0
	C_{3v}	3m	-	(0, 0, z)
	C_{3i}	$\bar{3}$	√	0
	C_3	3	-	(0, 0, z)
Orthorhombic	D_{2h}	mmm	√	0
	D_2	222	-	0
	D_{2v}	mm2	-	(0, 0, z)

POINT GROUPS

	Schönflies Notation	Hermann -Maugum	Inversion Center	Polar Vector
Monoclinic	C_{2h}	2/m	√	0
	C_S	m	-	(x, 0, z)
	C_2	2	-	(0, 0, z)
Triclinic	C_i	1	√	0
	C_1	$\bar{1}$	-	(x, y, z)

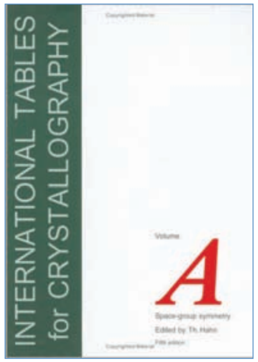
There are the 32 point group types.

Compound symmetry: screw axis and glide plane symmetry operations

The 230 unique space groups describing all possible crystal symmetries

FOR YOUR ADVANCED STUDY

International Tables for Crystallography, Volume A: Space Group Symmetry



Solid State Physics (Hardcover) by Gerald Burns