

Crystal Physics

The properties of solids

$$H = -\sum_i \frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_A \frac{\hbar^2}{2m_A} \nabla_A^2 - \sum_{i,A} \frac{Z_A e^2}{4\pi\epsilon_0 r_{iA}} + \sum_{i < j} \frac{e^2}{4\pi\epsilon_0 r_{ij}} + \sum_{A < B} \frac{Z_A Z_B e^2}{4\pi\epsilon_0 r_{AB}}$$



electronic band structure E vs. k

structure
bond potentials

phonon band structure ω vs. k

density of states

equilibrium properties
 c_v , free energies, bulk modulus,...

density of states

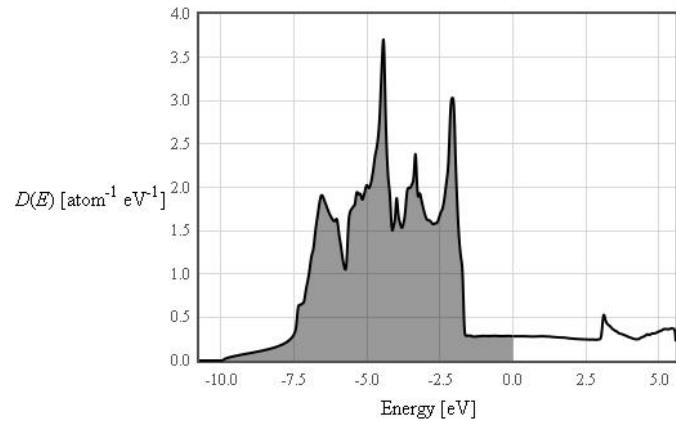
Boltzmann transport

optical
absorption

optical properties

Calculating free energies

Electronic component

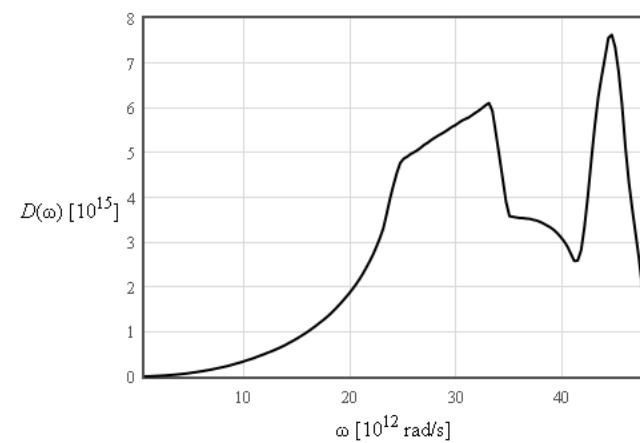


$$n = \int_{-\infty}^{\infty} \frac{D(E)}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)} dE$$

$$u = \int_{-\infty}^{\infty} \frac{ED(E)}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)} dE$$

Phonon component

$$u = \int_{-\infty}^{\infty} \frac{ED(E)}{\exp\left(\frac{E - \mu}{k_B T}\right) - 1} dE$$



Gibbs free energy

$$G(T, \mu, H, E, \sigma)$$

$$G = U - TS - \mu_i N_i - \sigma_{ij} \varepsilon_{ij} - E_k P_K - H_l M_l$$

$$S = - \left(\frac{\partial G}{\partial T} \right)_{\sigma, E, H, \mu} \quad N_i = - \left(\frac{\partial G}{\partial \mu_i} \right)_{T, E, H, \sigma} \quad \varepsilon_{ij} = - \left(\frac{\partial G}{\partial \sigma_{ij}} \right)_{T, E, H, \mu}$$

$$P_k = - \left(\frac{\partial G}{\partial E_k} \right)_{T, \mu, H, \sigma} \quad M_l = - \left(\frac{\partial G}{\partial H_l} \right)_{T, \mu, E, \sigma}$$

$$d\epsilon_{ij} = \left(\frac{\partial \epsilon_{ij}}{\partial \sigma_{kl}} \right) d\sigma_{kl} + \left(\frac{\partial \epsilon_{ij}}{\partial E_k} \right) dE_k + \left(\frac{\partial \epsilon_{ij}}{\partial H_l} \right) dH_l + \left(\frac{\partial \epsilon_{ij}}{\partial T} \right) dT$$

$$dP_i = \left(\frac{\partial P_i}{\partial \sigma_{kl}} \right) d\sigma_{kl} + \left(\frac{\partial P_i}{\partial E_k} \right) dE_k + \left(\frac{\partial P_i}{\partial H_l} \right) dH_l + \left(\frac{\partial P_i}{\partial T} \right) dT$$

$$dM_i = \left(\frac{\partial M_i}{\partial \sigma_{kl}} \right) d\sigma_{kl} + \left(\frac{\partial M_i}{\partial E_k} \right) dE_k + \left(\frac{\partial M_i}{\partial H_l} \right) dH_l + \left(\frac{\partial M_i}{\partial T} \right) dT$$

$$dS = \left(\frac{\partial S}{\partial \sigma_{kl}} \right) d\sigma_{kl} + \left(\frac{\partial S}{\partial E_k} \right) dE_k + \left(\frac{\partial S}{\partial H_l} \right) dH_l + \left(\frac{\partial S}{\partial T} \right) dT$$

1. Elastic deformation.
2. Reciprocal (or converse) piezo-electric effect.
3. Reciprocal (or converse) piezo-magnetic effect.
4. Thermal dilatation.
5. Piezo-electric effect.
6. Electric polarization.
7. Magneto-electric polarization.
8. Pyroelectricity.
9. Piezo-magnetic effect.
10. Reciprocal (or converse) magneto-electric polarization.
11. Magnetic polarization.
12. Pyromagnetism.
13. Piezo-caloric effect.
14. Electro-caloric effect.
15. Magneto-caloric effect.
16. Heat transmission.

Groups

Crystals can have symmetries: translation, rotation, reflection, inversion,...

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \alpha & \sin \alpha \\ 0 & -\sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Point symmetries can be represented by matrices.

All such matrices that bring the crystal into itself form the group of the crystal.

$$A, B \in G \quad AB \in G$$

32 point groups (one point remains fixed during transformation)

230 space groups

Cyclic groups

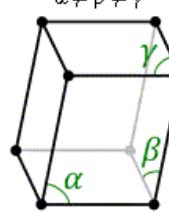
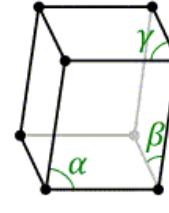
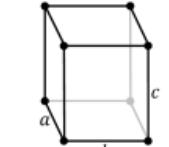
C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8

$$C_2 \quad E = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, C_2 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$C_4 \quad E = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, C_4 = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, C_2 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, C_4^3 = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$E = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, C_6 = \begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}, C_3 = \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}, C_2 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, C_3^2 = \begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}, C_6^5 = \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

The 32 Crystal Classes

Crystal system	Crystal Class	International symbol	Schoenflies symbol	Space groups	2-fold axes	3-fold axes	4-fold axes	6-fold axes	mirror planes	inversion	Examples	Number of symmetry elements
Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$ 	triclinic-pedial	1	C_1	1	-	-	-	-	-	n		1
	triclinic-pinacoidal	$\bar{1}$	$S_2 = C_i$	2	-	-	-	-	-	y		2
Monoclinic $a \neq b \neq c$ $\alpha \neq 90^\circ$, $\beta = \gamma = 90^\circ$ 	monoclinic-sphenoidal	2	C_2	3-5	1	-	-	-	-	n		2
	monoclinic-domatic	m	$C_{1h} = C_s$	6-9	-	-	-	-	1	n		2
	monoclinic-prismatic	$2/m$	C_{2h}	10-15	1	-	-	-	1	y		4
Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$ 	orthorhombic-disphenoidal	222	$V = D_2$	16-24	3	-	-	-	-	n		4
	orthorhombic-pyramidal	$mm2$	C_{2v}	25-46	1	-	-	-	2	n		4
											47: $\text{YBa}_2\text{Cu}_3\text{O}_{7.x}$	

Pyroelectricity

$$\pi_i = - \left(\frac{\partial^2 G}{\partial E_i \partial T} \right)$$

Pyroelectricity is described by a rank 1 tensor

$$\pi_i = \frac{\partial P_i}{\partial T}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} \pi_x \\ \pi_y \\ \pi_z \end{bmatrix} = \begin{bmatrix} \pi_x \\ \pi_y \\ -\pi_z \end{bmatrix} \Rightarrow \begin{bmatrix} \pi_x \\ \pi_y \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} \pi_x \\ \pi_y \\ \pi_z \end{bmatrix} = \begin{bmatrix} -\pi_x \\ -\pi_y \\ -\pi_z \end{bmatrix} \Rightarrow \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Pyroelectricity

Quartz, ZnO, LaTaO₃

example

Turmalin: point group 3m
for $\Delta T = 1^\circ\text{C}$,
 $\Delta E \sim 7 \cdot 10^4 \text{ V/m}$

Pyroelectrics have a spontaneous polarization. If it can be reversed by an electric field they are called Ferroelectrics (BaTiO₃)

Pyroelectrics are at Joanneum research to make infrared detectors (to detect humans).

10 Pyroelectric crystal classes: 1, 2, m, mm2, 3, 3m, 4, 4mm, 6, 6mm

Rank 2 Tensors

- Electric susceptibility
- Dielectric constant
- Magnetic susceptibility
- Thermal expansion
- Electrical conductivity
- Thermal conductivity
- Seebeck effect
- Peltier effect

Electric susceptibility

$$\chi_{ij} = - \left(\frac{\partial^2 G}{\partial E_i \partial E_j} \right)$$

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

$$\begin{bmatrix} P_x \\ P_y \\ P_z \end{bmatrix} = \begin{bmatrix} \chi_{xx} & \chi_{xy} & \chi_{xz} \\ \chi_{yx} & \chi_{yy} & \chi_{yz} \\ \chi_{zx} & \chi_{zy} & \chi_{zz} \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

Transforming P and E by a crystal symmetry must leave the susceptibility tensor unchanged

$$U\vec{P} = \chi U\vec{E}$$

$$U^{-1}U\vec{P} = U^{-1}\chi U\vec{E}$$

$$\chi = U^{-1}\chi U$$

If rotation by 180 about the z axis is a symmetry,

$$U = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad U^{-1} = U = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad U^{-1}\chi U = \begin{bmatrix} \chi_{xx} & \chi_{xy} & -\chi_{xz} \\ \chi_{yx} & \chi_{yy} & -\chi_{yz} \\ -\chi_{zx} & -\chi_{zy} & \chi_{zz} \end{bmatrix}$$

$$\chi_{xz} = \chi_{yz} = \chi_{zx} = \chi_{zy} = 0$$

Cubic crystals

All second rank tensors of cubic crystals reduce to constants

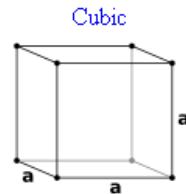
216: ZnS, GaAs, GaP, InAs

221: CsCl, cubic perovskite

225: Al, Cu, Ni, Ag, Pt, Au, Pb, NaCl

227: C, Si, Ge, spinel

229: Na, K, Cr, Fe, Nb, Mo, Ta



23	T	195-199		12
$m3$	T_h	200-206		24
432	O	207-214		24
$\bar{4}3m$	T_d	215-220	216: Zincblende, ZnS, GaAs, GaP, InAs, SiC	24
$m3m$	O_h	221-230	221: CsCl, cubic perovskite 225: fcc, Al, Cu, Ni, Ag, Pt, Au, Pb, γ -Fe, NaCl 227: diamond, C, Si,	48

$\begin{bmatrix} g_{11} & 0 & 0 \\ g_{11} & 0 & 0 \\ g_{11} & 0 & g_{11} \end{bmatrix}$

Multiferroics

simultaneously ferroelectric and ferromagnetic



If two magnetic sublattices have different charge, changing the magnetic field can change the polarization and changing the electric field can change the magnetization.

Material	ρ ($\Omega \cdot m$) at 20 °C	σ (S/m) at 20 °C	Temperature coefficient ^[note 1] (K^{-1})	Reference
Silver	1.59×10^{-8}	6.30×10^7	0.0038	[7][8]
Copper	1.68×10^{-8}	5.96×10^7	0.0039	[8]
Annealed copper ^[note 2]	1.72×10^{-8}	5.80×10^7		[citation needed]
Gold ^[note 3]	2.44×10^{-8}	4.10×10^7	0.0034	[7]
Aluminium ^[note 4]	2.82×10^{-8}	3.5×10^7	0.0039	[7]
Calcium	3.36×10^{-8}	2.98×10^7	0.0041	
Tungsten	5.60×10^{-8}	1.79×10^7	0.0045	[7]
Zinc	5.90×10^{-8}	1.69×10^7	0.0037	[9]
Nickel	6.99×10^{-8}	1.43×10^7	0.006	
Lithium	9.28×10^{-8}	1.08×10^7	0.006	
Iron	1.0×10^{-7}	1.00×10^7	0.005	[7]
Platinum	1.06×10^{-7}	9.43×10^6	0.00392	[7]
Tin	1.09×10^{-7}	9.17×10^6	0.0045	
Carbon steel (1010)	1.43×10^{-7}	6.99×10^6		[10]
Lead	2.2×10^{-7}	4.55×10^6	0.0039	[7]
Titanium	4.20×10^{-7}	2.38×10^6	X	
Grain oriented electrical steel	4.60×10^{-7}	2.17×10^6		[11]
Manganin	4.82×10^{-7}	2.07×10^6	0.000002	[12]
Constantan	4.9×10^{-7}	2.04×10^6	0.000008	[13]
Stainless steel ^[note 5]	6.9×10^{-7}	1.45×10^6		[14]
Mercury	9.8×10^{-7}	1.02×10^6	0.0009	[12]
Nichrome ^[note 6]	1.10×10^{-6}	9.09×10^5	0.0004	[7]
GaAs	5×10^{-7} to 10×10^{-3}	5×10^{-8} to 10^3		[15]
Carbon (amorphous)	5×10^{-4} to 8×10^{-4}	1.25 to 2×10^3	-0.0005	[7][16]
Carbon (graphite) ^[note 7]	$2.5e \times 10^{-6}$ to 5.0×10^{-6} //basal plane 3.0×10^{-3} \perp basal plane	2 to 3×10^5 //basal plane 3.3×10^2 \perp basal plane		[17]
Carbon (diamond) ^[note 8]	1×10^{12}	$\sim 10^{-13}$		[18]
Germanium ^[note 8]	4.6×10^{-1}	2.17	-0.048	[7][8]
Sea water ^[note 9]	2×10^{-1}	4.8		[19]
Electron	$2 \times 10^{-1} \text{ to } 2 \times 10^{-3}$	$2 \times 10^{-4} \text{ to } 2 \times 10^{-2}$		[citation needed]

```
_symmetry_equiv_pos_as_xyz
1 '-y+1/2, x+1/2, -z+1/2'
2 'y+1/2, -x+1/2, -z+1/2'
3 'y, x, -z'
4 '-y, -x, -z'
5 'y+1/2, -x+1/2, z+1/2'
6 '-y+1/2, x+1/2, z+1/2'
7 '-y, -x, z'
8 'y, x, z'
9 'x+1/2, -y+1/2, -z+1/2'
10 '-x+1/2, y+1/2, -z+1/2'
11 'x, y, -z'
12 '-x, -y, -z'
13 '-x+1/2, y+1/2, z+1/2'
14 'x+1/2, -y+1/2, z+1/2'
15 '-x, -y, z'
16 'x, y, z'
loop_
_atom_type_symbol
_atom_type_oxidation_number
Ti4+ 4
O2- -2
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_B_iso_or_equiv
_atom_site_occupancy
_atom_site_attached_hydrogens
Ti1 Ti4+ 2 a 0 0 0 . 1. 0
O1 O2- 4 f 0.30479(10) 0.30479(10) 0 . 1. 0
`
```

[view crystal in whole frame](#)

Rutile [TiO₂]

Structure Tetragonal

Space Group : *P4₂/mn*m (No. 136)

a=4.5937 Å *c*=2.9587 Å

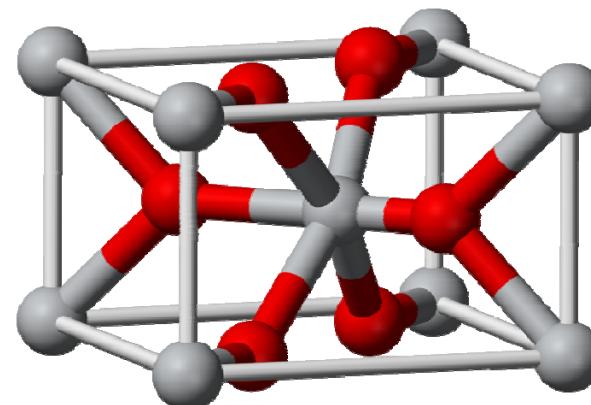
a=*b*=*g*=90.00

Z=2

Atomic Positional Parameters

Ti 2a 0.0000 0.0000 0.0000

O 4f 0.3048 0.3048 0.0000



Rank 3 Tensors

Piezoelectricity
Piezomagnetism
Hall effect
Nerst effect
Ettingshausen effect
Nonlinear electrical
susceptibility

Tensor notation

We need a way to represent 3rd and 4th rank tensors in 2-d.

1 1 → 1 1 2 → 6 1 3 → 5

2 2 → 2 2 3 → 4

3 3 → 3

rank 3

$g_{36} \rightarrow g_{312}$

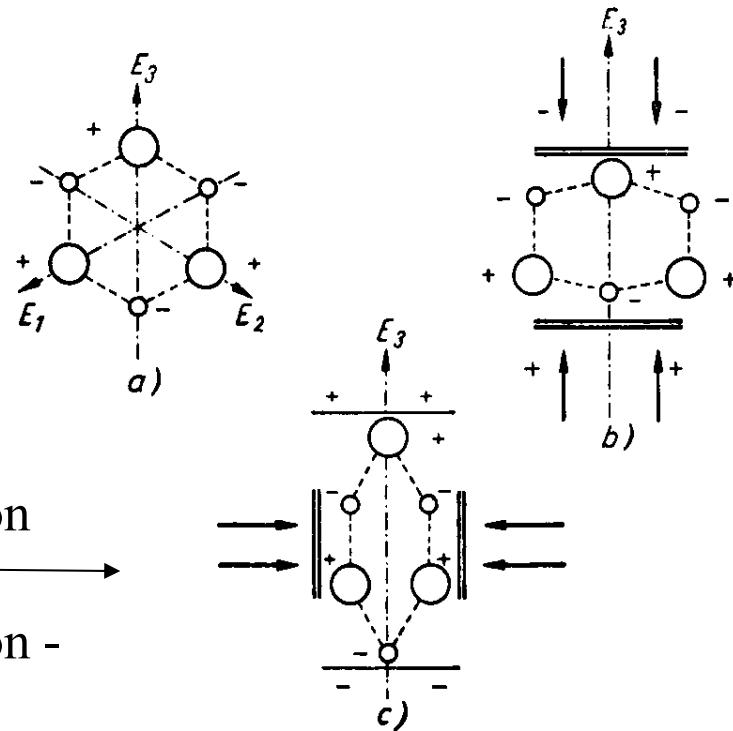
rank 4

$g_{14} \rightarrow g_{1123}$

Piezoelectricity

average position
+ is
average position -

average position
+ not
average position -



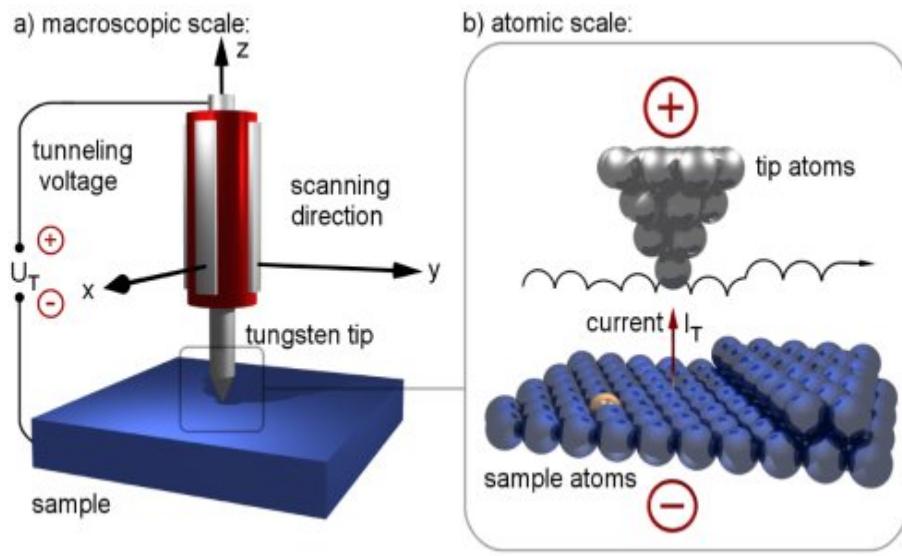
$$P_k = - \left(\frac{\partial G}{\partial E_k} \right)$$

$$\frac{\partial P_k}{\partial \sigma_{ij}} = - \left(\frac{\partial^2 G}{\partial E_k \partial \sigma_{ij}} \right) = d_{ijk}$$

Piezoelectricity (rank 3 tensor)

AFM's, STM's
Quartz crystal oscillators
Surface acoustic wave generators
Pressure sensors - Epcos
Fuel injectors - Bosch
Inkjet printers

No inversion symmetry



lead zirconate titanate ($\text{Pb}[\text{Zr}_x\text{Ti}_{1-x}]\text{O}_3$ $0 < x < 1$)
—more commonly known as PZT
barium titanate (BaTiO_3)
lead titanate (PbTiO_3)
potassium niobate (KNbO_3)
lithium niobate (LiNbO_3)
lithium tantalate (LiTaO_3)
sodium tungstate (Na_2WO_3)
 $\text{Ba}_2\text{NaNb}_5\text{O}_5$
 $\text{Pb}_2\text{KNb}_5\text{O}_{15}$

Piezoelectric crystal classes: 1, 2, m, 222, mm2, 4, -4, 422, 4mm, -42m, 3, 32, 3m, 6, -6, 622, 6mm, -62m, 23, -43m

Nonlinear optics

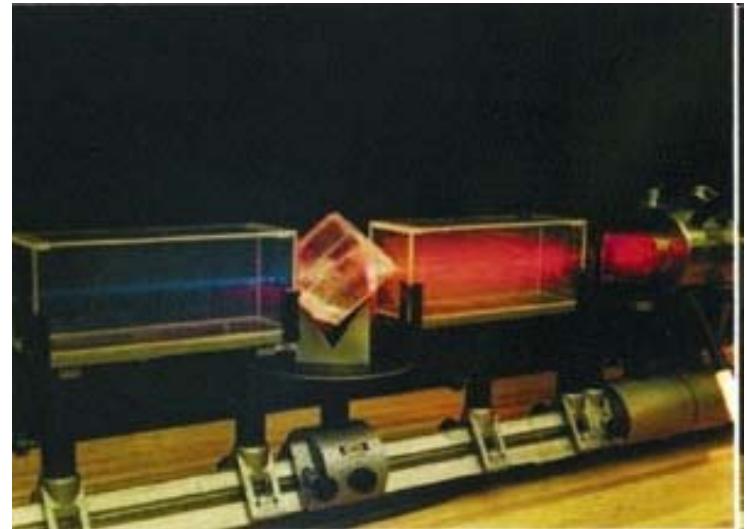
Period doubling crystals

no inversion symmetry

$$P = \chi^{(1)}E + \chi^{(2)}E^2 + \chi^{(3)}E^3 + \dots$$

$$P_i = \frac{-\partial^2 G}{\partial E_i \partial E_j} E_j + \frac{1}{2} \frac{-\partial^3 G}{\partial E_i \partial E_j \partial E_k} E_j E_k + \dots$$

$$\cos^2(\omega t) = \frac{1}{2}(1 + \cos(2\omega t))$$



806 nm light : lithium iodate (LiIO_3)

860 nm light : potassium niobate (KNbO_3)

980 nm light : KNbO_3

1064 nm light : monopotassium phosphate (KH_2PO_4 , KDP), lithium triborate (LBO).

1300 nm light : gallium selenide (GaSe)

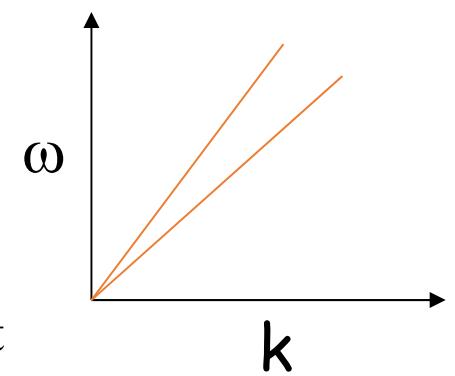
1319 nm light : KNbO_3 , BBO, KDP, lithium niobate (LiNbO_3), LiIO_3

Birefringence (Doppelbrechung)



Calcite

Two indices of refraction



<http://en.wikipedia.org/wiki/Birefringent>

Birefringence

Electric susceptibility

[edit]

In an [isotropic](#) and [linear](#) medium, this polarisation field \mathbf{P} is proportional to and parallel to the electric field \mathbf{E} :

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

where χ is the [electric susceptibility](#) of the medium. The relation between \mathbf{D} and \mathbf{E} is thus:

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

where

$$\varepsilon = \varepsilon_0 (1 + \chi)$$

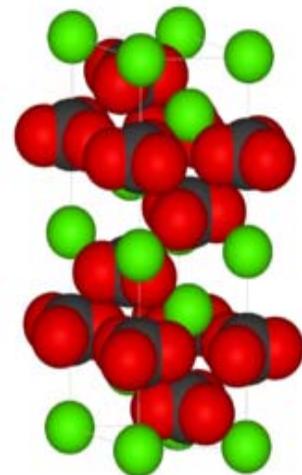
is the [dielectric constant](#) of the medium. The value $1 + \chi$ is called the *relative permittivity* of the medium, and is related to the [refractive index](#) n , for non-magnetic media, by

$$n = \sqrt{1 + \chi}$$

Birefringence



Calcite



name	international	Schoenflies	examples
rhombohedral holohedral	$\bar{3}m$	D_{3d}	calcite, corundum, hematite
rhombohedral hemimorphic	$3m$	C_{3v}	tourmaline, alunite
rhombohedral tetartohedral	$\bar{3}$	S_6	dolomite, ilmenite
trapezohedral	32	D_3	quartz, cinnabar
rhombohedral tetartohedral	3	C_3	none verified

Rhombohedral crystal system

From Wikipedia, the free encyclopedia
 (Redirected from [Trigonal crystal system](#))



An example
crystals, que

name	international	Schoenflies	examples
rhombohedral holohedral	$\bar{3}m$	D_{3d}	calcite, corundum, hematite
rhombohedral hemimorphic	$3m$	C_{3v}	tourmaline, alunite
rhombohedral tetartohedral	$\bar{3}$	S_6	dolomite, ilmenite
trapezohedral	32	D_3	quartz, cinnabar
rhombohedral tetartohedral	3	C_3	none verified

In [crystallography](#), the **rhombohedral** (or **trigonal**) [crystal system](#) is one of the seven [lattice point groups](#), named after the two-dimensional [rhombus](#). A [crystal](#) system is described by three basis [vectors](#). In the rhombohedral system, the crystal is described by vectors of [equal length](#), of which all three are not mutually [orthogonal](#). The **rhombohedral system** can be thought of as the [cubic system](#) stretched [diagonally](#) along a body. $a = b = c$; $\alpha, \beta, \gamma \neq 90^\circ$. In some classification schemes, the **rhombohedral system** is grouped into a larger [hexagonal system](#).

	$\bar{3}$	$S_6 = C_{6i}$	147-148	6	$\begin{bmatrix} g_{11} & 0 & 0 \\ g_{11} & 0 & 0 \\ & & g_{33} \end{bmatrix}$
	32	D_3	149-155	6	
	$3m$	C_{3v}	156-161	6	
	$\bar{3}m$	D_{3d}	162-167	12	

Rhombohedral = Trigonal

Optical effects

$$P_i = P_i^0 + \frac{\partial P_i}{\partial E_j} E_j + \frac{\partial^2 P_i}{\partial E_j \partial E_k} E_j E_k + \frac{\partial^2 P_i}{\partial E_j \partial E_k \partial E_l} E_j E_k E_l + \dots$$

↑
spontaneous
polarization

↑
 E_k DC
Pockels effect

↑
 E_k, E_l DC
Kerr effect

$$P_i = \frac{\partial^2 P_i}{\partial E_j \partial H_k} E_j H_k + \frac{\partial^2 P_i}{\partial E_j \partial H_k \partial H_l} E_j H_k H_l + \dots$$

↑
 H_k DC
Faraday effect

↑
 H_k, H_l DC
Cotton–Mouton effect

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Chapter 1.6. Classical linear crystal optics¹

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Chapter 1.7. Nonlinear optical properties

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Electrostriction

$$\frac{\partial P_k}{\partial \sigma_{ij}} = \frac{\partial \epsilon_{ij}}{\partial E_k} - \left(\frac{\partial^2 G}{\partial E_k \partial \sigma_{ij}} \right) = d_{ijk}$$

$$\epsilon_{ij} = d_{ijk} E_k + Q_{ijkl} E_k E_l + \dots$$



Rank 4 Tensors

Stiffness tensor

Compliance tensor

Piezoelectricity

Electrostriction

Magnetostriction

How the Seebeck effect depends on stress

How the electric susceptibility depends on stress

How the magnetic susceptibility depends on stress

Nonlinear electric susceptibility

Nonlinear magnetic susceptibility

Symmetric and asymmetric tensors

$$-\left(\frac{\partial^2 G}{\partial E_j \partial E_k}\right) = \frac{\partial P_k}{\partial E_j} = \chi_{kj} = -\left(\frac{\partial^2 G}{\partial E_k \partial E_j}\right) = \frac{\partial P_j}{\partial E_k} = \chi_{jk}$$

Symmetric
electric susceptibility
magnetic susceptibility
electrical conductivity
thermal conductivity
stiffness tensor

Asymmetric
Seebeck effect
Peltier effect
piezoconductivity