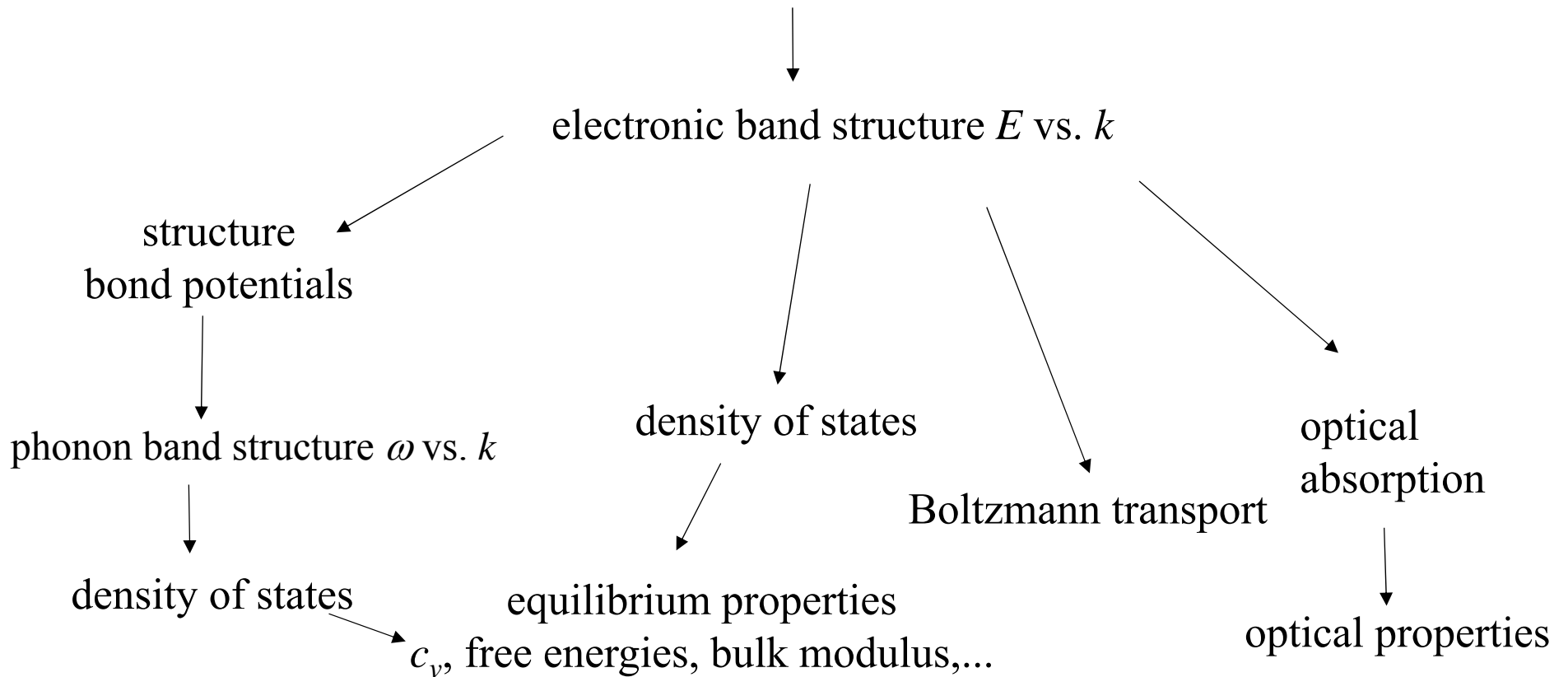


25. Crystal Physics

Jan. 20, 2020

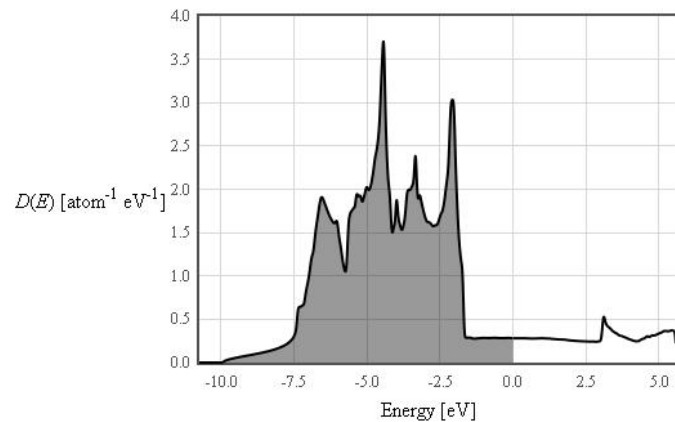
The properties of solids

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



Calculating free energies

Electronic component

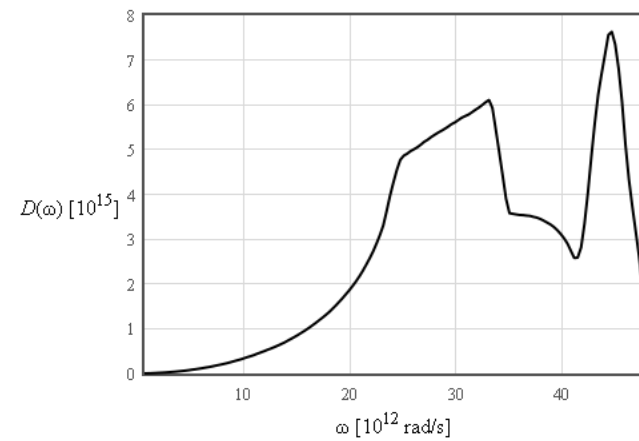


$$n = \int_{-\infty}^{\infty} \frac{D(E)}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)} dE$$

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

Phonon component

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



<http://it.iucr.org>

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International Tables for Crystallography Volume D: Physical properties of crystals

Second online edition (2013) ISBN: 978-1-118-76229-5 doi: 10.1107/97809553602060000113

Edited by **A. Authier**

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Statistical Physics

Microcanonical Ensemble: Internal energy is expressed in terms of extrinsic quantities $U(S, M, P, \varepsilon, N)$.

$$dU = \frac{\partial U}{\partial S} dS + \frac{\partial U}{\partial \varepsilon_{ij}} d\varepsilon_{ij} + \frac{\partial U}{\partial P_K} dP_K + \frac{\partial U}{\partial M_l} dM_l$$

$$dU = TdS + \sigma_{ij}d\varepsilon_{ij} + E_k dP_K + H_l dM_l$$

The normal modes must be solved for in the presence of electric and magnetic fields.

Internal energy in an electric field

In an electric field, if the dipole moment is changed, the change of the energy is,

$$\Delta U = \vec{E} \cdot \Delta \vec{P}$$

Using Einstein notation

$$dU = E_k dP_k$$

This is part of the total derivative of U

$$E_k = \frac{\partial U}{\partial P_k}$$

$$dU = TdS + \sigma_{ij} d\varepsilon_{ij} + E_k dP_k + H_l dM_l$$

Helmholtz free energy

Canonical ensemble: At constant temperature, make a Legendre transformation to the Helmholtz free energy.

$$F = U - TS$$

$$F(T, N, M, P, \varepsilon)$$

$$dF = \frac{\partial F}{\partial T} dT + \frac{\partial F}{\partial N_i} dN_i + \frac{\partial F}{\partial \varepsilon_{ij}} d\varepsilon_{ij} + \frac{\partial F}{\partial P_k} dP_k + \frac{\partial F}{\partial M_l} dM_l$$

$$dF = dU - TdS - SdT$$

$$dF = -SdT + \mu_i dN_i + \sigma_{ij} d\varepsilon_{ij} + E_k dP_k + H_l dM_l$$

$$S = -\left(\frac{\partial F}{\partial T}\right)_{N, M, P, \varepsilon} \quad \mu_i = \left(\frac{\partial F}{\partial N_i}\right)_{T, M, P, \varepsilon, N_{j \neq i}} \quad \sigma_{ij} = \left(\frac{\partial F}{\partial \varepsilon_{ij}}\right)_{N, M, P, T}$$

$$E_k = \left(\frac{\partial F}{\partial P_k}\right)_{N, M, T, \varepsilon} \quad H_l = \left(\frac{\partial F}{\partial M_l}\right)_{N, T, P, \varepsilon}$$

Gibbs free energy

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

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

$$dU = TdS + \mu_i dN_i + \sigma_{ij} d\varepsilon_{ij} + E_k dP_k + H_l dM_l$$

$$dG = -SdT - N_i d\mu_i - \varepsilon_{ij} d\sigma_{ij} - P_k dE_k - M_l dH_l$$

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

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

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

$$\begin{aligned}
d\epsilon_{ij} &= \left(\frac{\partial \epsilon_{ij}}{\partial \sigma_{kl}}\right) d\sigma_{kl} + \left(\frac{\partial \epsilon_{ij}}{\partial E_k}\right) dE_k + \left(\frac{\partial \epsilon_{ij}}{\partial H_l}\right) dH_l + \left(\frac{\partial \epsilon_{ij}}{\partial T}\right) dT \\
dP_i &= \left(\frac{\partial P_i}{\partial \sigma_{kl}}\right) d\sigma_{kl} + \left(\frac{\partial P_i}{\partial E_k}\right) dE_k + \left(\frac{\partial P_i}{\partial H_l}\right) dH_l + \left(\frac{\partial P_i}{\partial T}\right) dT \\
dM_i &= \left(\frac{\partial M_i}{\partial \sigma_{kl}}\right) d\sigma_{kl} + \left(\frac{\partial M_i}{\partial E_k}\right) dE_k + \left(\frac{\partial M_i}{\partial H_l}\right) dH_l + \left(\frac{\partial M_i}{\partial T}\right) dT \\
dS &= \left(\frac{\partial S}{\partial \sigma_{kl}}\right) d\sigma_{kl} + \left(\frac{\partial S}{\partial E_k}\right) dE_k + \left(\frac{\partial S}{\partial H_l}\right) dH_l + \left(\frac{\partial S}{\partial T}\right) dT
\end{aligned}$$

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.

Direct and reciprocal effects (Maxwell relations)

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

$$-\left(\frac{\partial^2 G}{\partial \sigma_{ij} \partial H_l}\right) = \left(\frac{\partial M_l}{\partial \sigma_{ij}}\right) = -\left(\frac{\partial^2 G}{\partial H_l \partial \sigma_{ij}}\right) = \left(\frac{\partial \epsilon_{ij}}{\partial H_l}\right) = q_{lij}$$

$$-\left(\frac{\partial^2 G}{\partial E_k \partial H_l}\right) = \left(\frac{\partial M_l}{\partial E_k}\right) = -\left(\frac{\partial^2 G}{\partial H_l \partial E_k}\right) = \left(\frac{\partial P_k}{\partial H_l}\right) = \lambda_{lk}$$

$$-\left(\frac{\partial^2 G}{\partial \sigma_{ij} \partial T}\right) = \left(\frac{\partial S}{\partial \sigma_{ij}}\right) = -\left(\frac{\partial^2 G}{\partial T \partial \sigma_{ij}}\right) = \left(\frac{\partial \epsilon_{ij}}{\partial T}\right) = \alpha_{ij}$$

$$-\left(\frac{\partial^2 G}{\partial T \partial E_k}\right) = \left(\frac{\partial P_k}{\partial T}\right) = -\left(\frac{\partial^2 G}{\partial E_k \partial T}\right) = \left(\frac{\partial S}{\partial E_k}\right) = p_k$$

$$-\left(\frac{\partial^2 G}{\partial T \partial H_l}\right) = \left(\frac{\partial M_l}{\partial T}\right) = -\left(\frac{\partial^2 G}{\partial H_l \partial T}\right) = \left(\frac{\partial S}{\partial H_l}\right) = m_l.$$

Useful to check for errors in experiments or calculations

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.

Maxwell relations

$$\begin{aligned} + \left(\frac{\partial T}{\partial V} \right)_S &= - \left(\frac{\partial P}{\partial S} \right)_V = \frac{\partial^2 U}{\partial S \partial V} \\ + \left(\frac{\partial T}{\partial P} \right)_S &= + \left(\frac{\partial V}{\partial S} \right)_P = \frac{\partial^2 H}{\partial S \partial P} \\ + \left(\frac{\partial S}{\partial V} \right)_T &= + \left(\frac{\partial P}{\partial T} \right)_V = - \frac{\partial^2 F}{\partial T \partial V} \\ - \left(\frac{\partial S}{\partial P} \right)_T &= + \left(\frac{\partial V}{\partial T} \right)_P = \frac{\partial^2 G}{\partial T \partial P} \end{aligned}$$

Useful to check for errors in experiments or calculations

Groups

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

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

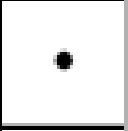
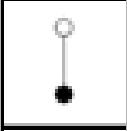

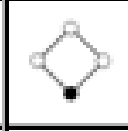
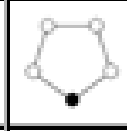
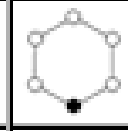
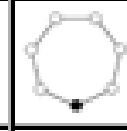
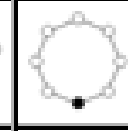
Symmetries can be represented by matrices.

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

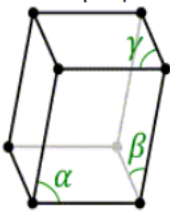
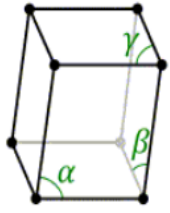
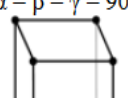
$$C_2 \quad E = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, C_2 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

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

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

http://en.wikipedia.org/wiki/Cyclic_group

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: P1	-	-	-	-	-	n		1
	triclinic-pinacoidal	$\bar{1}$	$S_2 = C_i$	2: $P\bar{1}$	-	-	-	-	-	y		2
Monoclinic $a \neq b \neq c$ $\alpha \neq 90^\circ$, $\beta = \gamma = 90^\circ$ 	monoclinic-sphenoidal	2	C_2	3: P2, 4: P2 ₁ , 5: C2	1	-	-	-	-	n		2
	monoclinic-domatic	m	$C_{1h} = C_s$	6: Pm, 7: Pc, 8: Cm, 9: Cc	-	-	-	-	1	n		2
	monoclinic-prismatic	$\frac{2}{m}$	C_{2h}	10: P2/m, 11: P2 ₁ /m, 12: C2/m, 13: P2/c, 14: P2 ₁ /c, 15: C2/c	1	-	-	-	1	y		4
Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$ 	orthorhombic-disphenoidal	222	$V = D_2$	16: P222, 17: P222 ₁ , 18: P2 ₁ 2 ₁ 2, 19: P2 ₁ 2 ₁ 2 ₁ , 20: C222 ₁ , 21: C222, 22: F222, 23: I222, 24: I2 ₁ 2 ₁ 2 ₁	3	-	-	-	-	n		4
	orthorhombic-pyramidal	$mm2$	C_{2v}	25: Pmm2, 26: Pmc2 ₁ , 27: Pcc2, 28: Pma2, 29: Pca2 ₁ , 30: Pnc2, 31: Pmn2 ₁ , 32: Pba2, 33: Pna2 ₁ , 34: Pnn2 35: Cmm2, 36: Cmc2 ₁ , 37: Ccc2, 38: Amm2, 39: Aem2, 40: Ama2, 41: Aea2, 42: Fmm2, 43: Fdd2, 44: Imm2, 45: Iba2, 46: Ima2	1	-	-	-	2	n		4

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

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

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

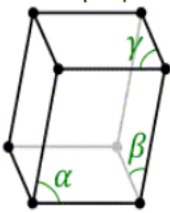
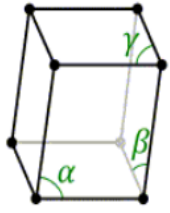
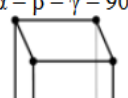
$$\chi = U^{-1}\chi U$$

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

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

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

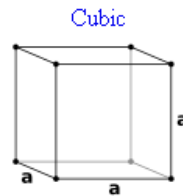
The 32 Crystal Classes

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: P1	-	-	-	-	-	n		1
	triclinic-pinacoidal	$\bar{1}$	$S_2 = C_i$	2: $P\bar{1}$	-	-	-	-	-	y		2
Monoclinic $a \neq b \neq c$ $\alpha \neq 90^\circ$, $\beta = \gamma = 90^\circ$ 	monoclinic-sphenoidal	2	C_2	3: P2, 4: P2 ₁ , 5: C2	1	-	-	-	-	n		2
	monoclinic-domatic	m	$C_{1h} = C_s$	6: Pm, 7: Pc, 8: Cm, 9: Cc	-	-	-	-	1	n		2
	monoclinic-prismatic	$\frac{2}{m}$	C_{2h}	10: P2/m, 11: P2 ₁ /m, 12: C2/m, 13: P2/c, 14: P2 ₁ /c, 15: C2/c	1	-	-	-	1	y		4
Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$ 	orthorhombic-disphenoidal	222	$V = D_2$	16: P222, 17: P222 ₁ , 18: P2 ₁ 2 ₁ 2, 19: P2 ₁ 2 ₁ 2 ₁ , 20: C222 ₁ , 21: C222, 22: F222, 23: I222, 24: I2 ₁ 2 ₁ 2 ₁	3	-	-	-	-	n		4
	orthorhombic-pyramidal	$mm2$	C_{2v}	25: Pmm2, 26: Pmc2 ₁ , 27: Pcc2, 28: Pma2, 29: Pca2 ₁ , 30: Pnc2, 31: Pmn2 ₁ , 32: Pba2, 33: Pna2 ₁ , 34: Pnn2 35: Cmm2, 36: Cmc2 ₁ , 37: Ccc2, 38: Amm2, 39: Aem2, 40: Ama2, 41: Aea2, 42: Fmm2, 43: Fdd2, 44: Imm2, 45: Iba2, 46: Ima2	1	-	-	-	2	n		4

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
$m\bar{3}$	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
$m\bar{3}m$	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

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

Material	↕	ρ ($\Omega\cdot\text{m}$) 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]		2.5×10^{-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]
Sea water ^[note 10]		2.4×10^{-1} to 2.4×10^{-3}	5.4×10^{-4} to 5.4×10^{-2}		[citation needed]

Rutile

```

From Wikipedia, the free encyclopedia
_symmetry_equiv_pos_as_xyz
1 '-y+1/2, x+1/2, -z+1/2'
Rt 2 'y+1/2, -x+1/2, -z+1/2'
Rt 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'
Rt 7 '-y, -x, z'
8 'y, x, z'
pa 9 'x+1/2, -y+1/2, -z+1/2'
op 10 '-x+1/2, y+1/2, -z+1/2'
Na 11 'x, y, -z'
th 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

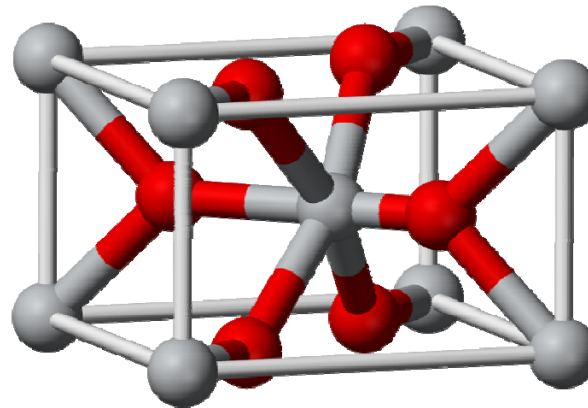
```

re known:

al mineral of pseudo-octahedral habit

own crystal, and also exhibits a
it is useful for the manufacture of certain
avelengths up to about 4.5µm.

d **tantalum**. Rutile derives its name from
mens when viewed by transmitted light.



1 high-temperature and high-pressure
s.

able polymorph of TiO₂ at all
energy than metastable phases of
e transformation of the metastable TiO

Rutile



Wine-red rutile crystals from Binn Valley in
Switzerland (Size: 2.0 x 1.6 x 0.8 cm)

General

Category	Oxide minerals
Formula (repeating unit)	TiO ₂
Strunz classification	04.DB.05
Crystal symmetry	Tetragonal ditetragonal dipyramidal H-M symbol: (4/m 2/m 2/m) Space group: P 4/mnm
Unit cell	a = 4.5937 Å, c = 2.9587 Å; Z = 2

Identification

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.

$$1\ 1 \rightarrow 1 \quad 1\ 2 \rightarrow 6 \quad 1\ 3 \rightarrow 5$$

$$2\ 2 \rightarrow 2 \quad 2\ 3 \rightarrow 4$$

$$3\ 3 \rightarrow 3$$

rank 3

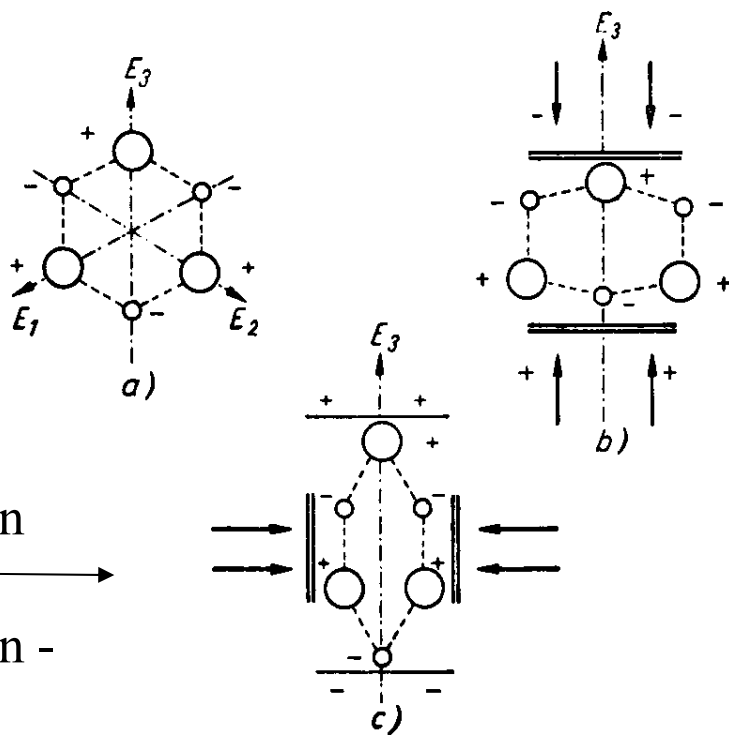
$$g_{36} \rightarrow g_{312}$$

rank 4

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

Piezoelectricity

average position
+ is
average position -



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

average position
+ not
average position -

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

Piezoelectricity (rank 3 tensor)

AFM's, STM's

Quartz crystal oscillators

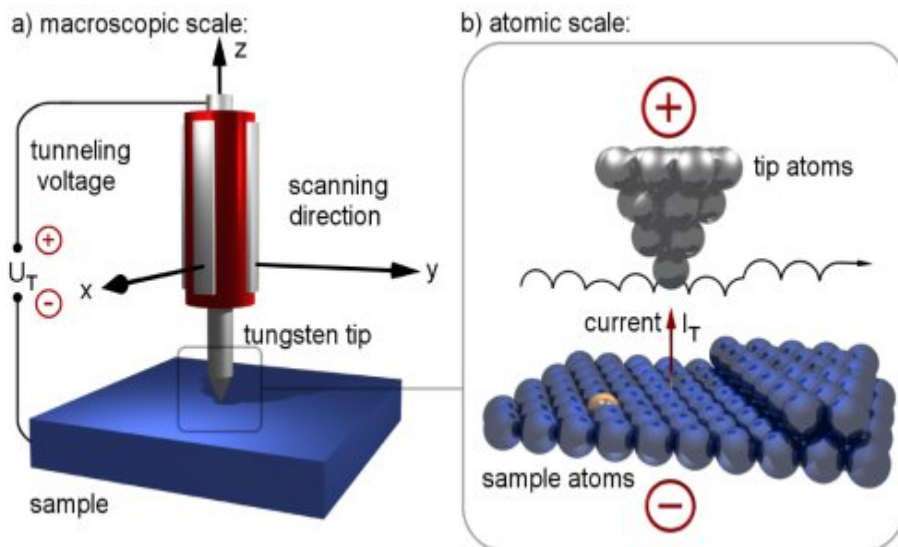
Surface acoustic wave generators

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)

$\text{Ba}_2\text{NaNb}_5\text{O}_{15}$

$\text{Pb}_2\text{KNb}_5\text{O}_{15}$

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

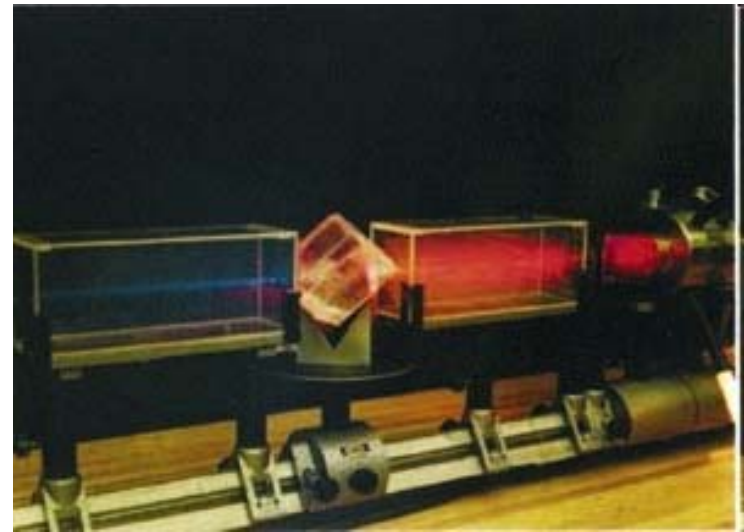
Period doubling crystals

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

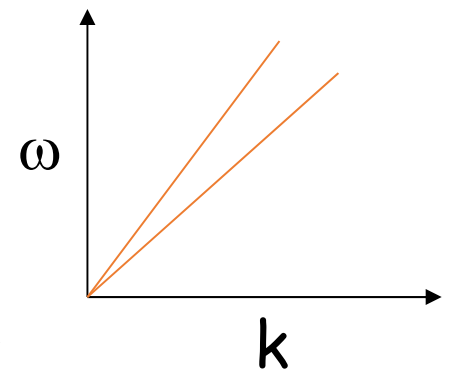
Birefringence (Doppelbrechung)



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} :

$$\mathbf{P} = \chi\epsilon_0\mathbf{E}$$

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

$$\mathbf{D} = \epsilon_0\mathbf{E} + \chi\epsilon_0\mathbf{E} = \epsilon_0(1 + \chi)\mathbf{E} = \epsilon\mathbf{E}$$

where

$$\epsilon = \epsilon_0(1 + \chi)$$

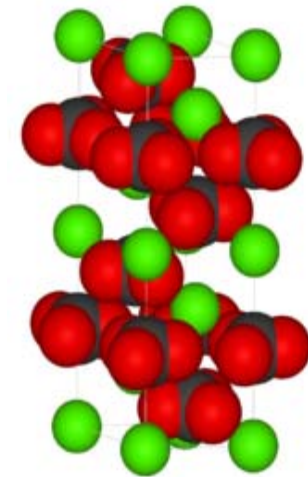
is the [dielectric constant](#) of the medium. The value $1+\chi$ is called the *relative permittivity* of the medium, and is related to the [refractive index](#) n , for non-magnetic media, by

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

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](#))

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](#).



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

Rhombohedral = Trigonal

	$\bar{3}$	$S_6 = C_{6i}$	147-148	6
	32	D_3	149-155	6
	$3m$	C_{3v}	156-161	6
	$\bar{3}m$	D_{3d}	162-167	12

$$\begin{bmatrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{bmatrix}$$

Electrostriction

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

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

piezoelectricity



Electrostriction



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