22. Crystal Physics

Jan. 7, 2018

Hall effect / Nerst effect

$$\vec{j}_{\mathrm{elec}} = \frac{e}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial\mu}\nabla_{\vec{k}}E(\vec{k})\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\nabla_{\vec{r}}\tilde{\mu}+\frac{E(\vec{k})-\mu}{T}\nabla_{\vec{r}}T+\frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k})\times\vec{B}\right)\right)d^3k.$$

$$f(\vec{k},\vec{r}) = f_0(\vec{k},\vec{r}) - \tau(\vec{k})\left(\frac{1}{\hbar}\vec{F}_{\mathrm{ext}}\cdot\nabla_{\vec{k}}f(\vec{k},\vec{r}) + \vec{v}\cdot\nabla_{\vec{r}}f(\vec{k},\vec{r})\right).$$

$$f(\vec{k},\vec{r}) \approx f_0(\vec{k},\vec{r}) - \tau(\vec{k})\left(\frac{1}{\hbar}\vec{F}_{\mathrm{ext}}\cdot\nabla_{\vec{k}}f_0(\vec{k},\vec{r}) + \vec{v}\cdot\nabla_{\vec{r}}f_0(\vec{k},\vec{r})\right).$$

Crystal Physics

Crystal physics explains what effects the symmetries of the crystal have on observable quantities.

An Introduction to Crystal Physics Ervin Hartmann
http://ww1.iucr.org/comm/cteach/pamphlets/18/index.html

International Tables for Crystallography
http://it.iucr.org/

Kittel chapter 3: elastic strain

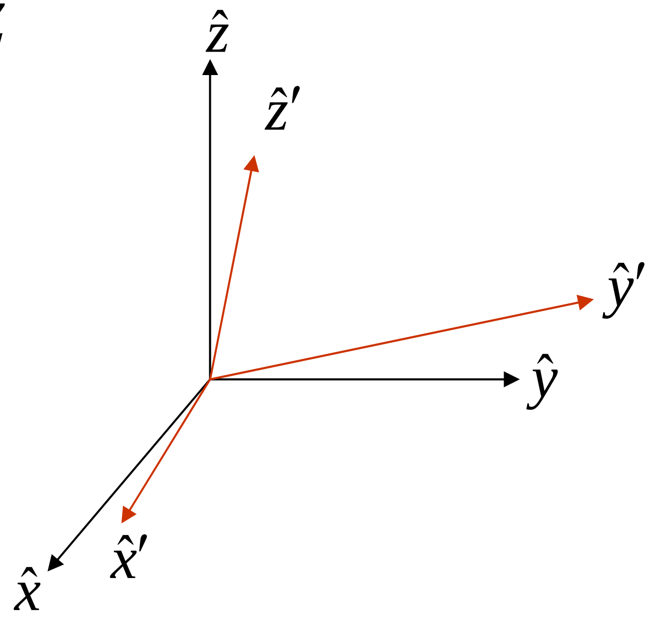
Strain

A distortion of a material is described by the strain matrix

$$x' = (1+\varepsilon_{xx})\hat{x} + \varepsilon_{xy}\hat{y} + \varepsilon_{xz}\hat{z}$$

$$y' = \varepsilon_{yx}\hat{x} + (1+\varepsilon_{yy})\hat{y} + \varepsilon_{yz}\hat{z}$$

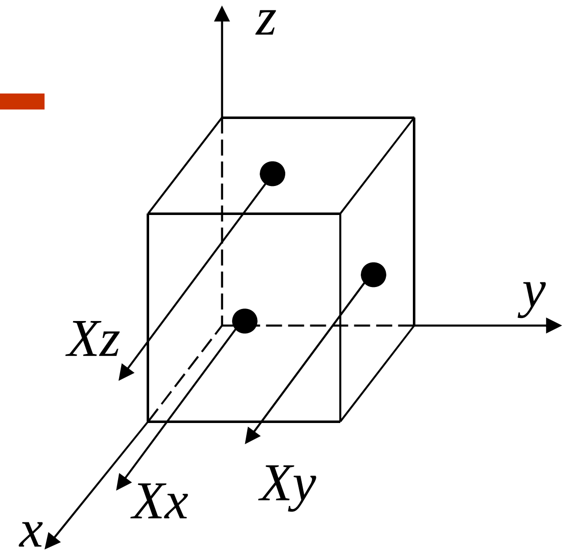
$$z' = \varepsilon_{zx}\hat{x} + \varepsilon_{zy}\hat{y} + (1+\varepsilon_{zz})\hat{z}$$



Stress

9 forces describe the stress

Xx, Xy, Xz, Yx, Yy, Yz, Zx, Zy, Zz



Xx is a force applied in the *x*-direction to the plane normal to *x*

Xy is a sheer force applied in the *x*-direction to the plane normal to *y*

stress tensor:

$$\sigma = \begin{bmatrix} \frac{X_x}{A_x} & \frac{X_y}{A_y} & \frac{X_z}{A_z} \\ \frac{Y_x}{A_x} & \frac{Y_y}{A_y} & \frac{Y_z}{A_z} \\ \frac{Z_x}{A_x} & \frac{Z_y}{A_y} & \frac{Z_z}{A_z} \end{bmatrix}$$

Stress is force/m^2

Stress and Strain

$$\varepsilon_{ij} = s_{ijkl}\sigma_{kl}$$

The stress - strain relationship is described by a rank 4 stiffness tensor. The inverse of the stiffness tensor is the compliance tensor.

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$$

Einstein convention: sum over repeated indices.

$$\varepsilon_{xx} = s_{xxxx}\sigma_{xx} + s_{xxxy}\sigma_{xy} + s_{xxxz}\sigma_{xz} + s_{xxyx}\sigma_{yx} + s_{xxyy}\sigma_{yy}$$

$$+ s_{xxyz}\sigma_{yz} + s_{xxzx}\sigma_{zx} + s_{xxzy}\sigma_{zy} + s_{xxzz}\sigma_{zz}$$

Statistical Physics

Microcannonical 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

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

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

Statistical Physics

Microcannonical Ensemble: Internal energy is expressed in terms of extrinsic quantities *U*(*S*, *M*, *P*, ε, *N*). $\varepsilon_{ij} \Rightarrow V\varepsilon_{ij}$

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

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

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

$F = U - TS$

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

Make a Legendre transformation to the Gibbs potential $G(T, H, E, \sigma)$

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

Helmholtz free energy

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

$$F = U - TS$$

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

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

$$dF = dU - TdS - SdT$$

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

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

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

Gibbs free energy

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

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

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

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

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

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

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

$$d\epsilon_{ij} = \underset{1}{\left(\frac{\partial \epsilon_{ij}}{\partial \sigma_{kl}}\right)} d\sigma_{kl} + \underset{2}{\left(\frac{\partial \epsilon_{ij}}{\partial E_k}\right)} dE_k + \underset{3}{\left(\frac{\partial \epsilon_{ij}}{\partial H_l}\right)} dH_l + \underset{4}{\left(\frac{\partial \epsilon_{ij}}{\partial T}\right)} dT$$

$$dP_i = \underset{5}{\left(\frac{\partial P_i}{\partial \sigma_{kl}}\right)} d\sigma_{kl} + \underset{6}{\left(\frac{\partial P_i}{\partial E_k}\right)} dE_k + \underset{7}{\left(\frac{\partial P_i}{\partial H_l}\right)} dH_l + \underset{8}{\left(\frac{\partial P_i}{\partial T}\right)} dT$$

$$dM_i = \underset{9}{\left(\frac{\partial M_i}{\partial \sigma_{kl}}\right)} d\sigma_{kl} + \underset{10}{\left(\frac{\partial M_i}{\partial E_k}\right)} dE_k + \underset{11}{\left(\frac{\partial M_i}{\partial H_l}\right)} dH_l + \underset{12}{\left(\frac{\partial M_i}{\partial T}\right)} dT$$

$$dS = \underset{13}{\left(\frac{\partial S}{\partial \sigma_{kl}}\right)} d\sigma_{kl} + \underset{14}{\left(\frac{\partial S}{\partial E_k}\right)} dE_k + \underset{15}{\left(\frac{\partial S}{\partial H_l}\right)} dH_l + \underset{16}{\left(\frac{\partial S}{\partial T}\right)} dT$$

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.

http://www.iucr.org/education/pamphlets/18

Direct and reciprocal effects (Maxwell relations)

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

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

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

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

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

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

Useful to check for errors in experiments or calculations

Multiferroics

simultaneously ferroelectric and ferromagnetic

$BiFeO_3$

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

$$+\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V = \frac{\partial^2 U}{\partial S \partial V}$$

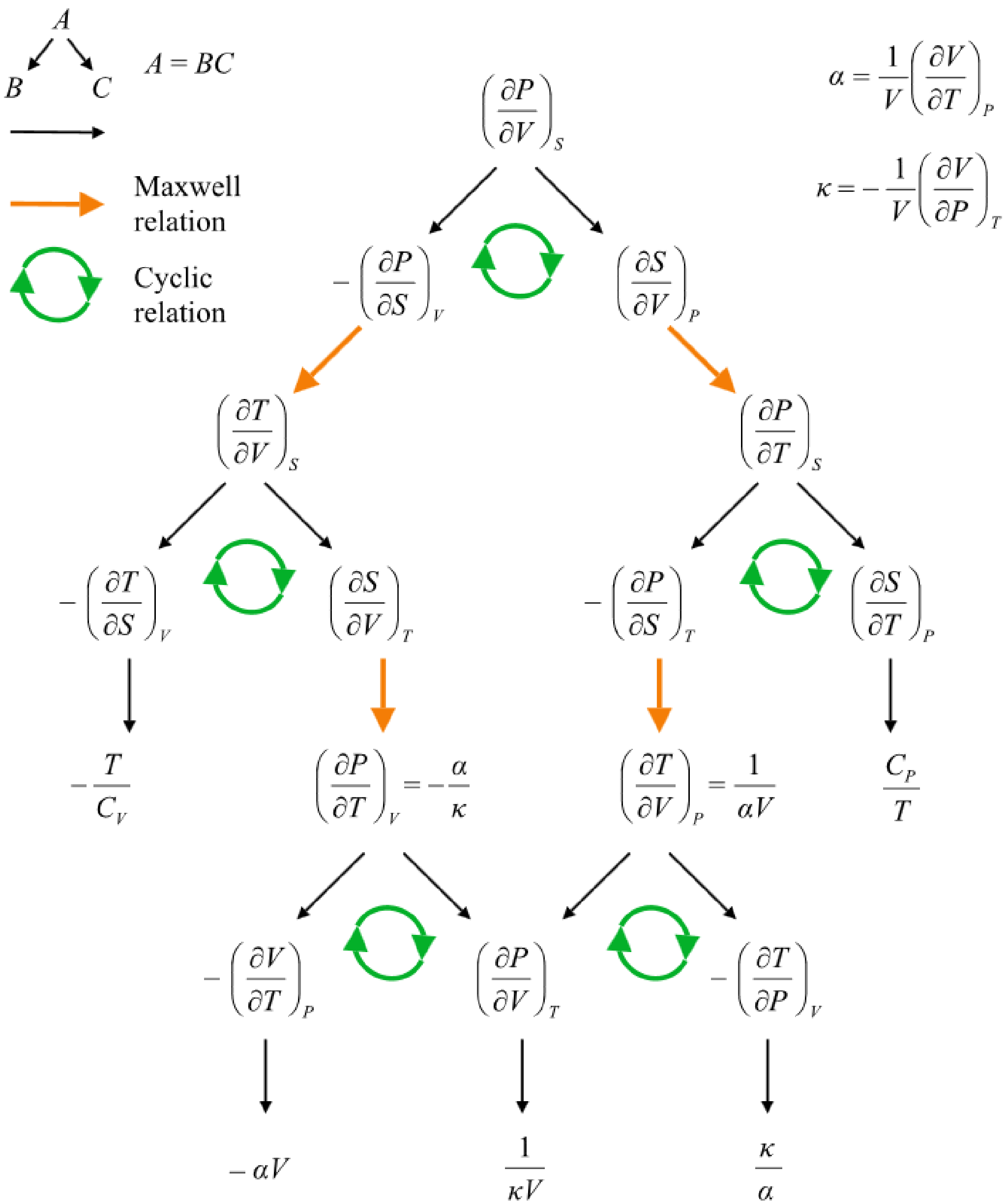
$$+\left(\frac{\partial T}{\partial P}\right)_S = +\left(\frac{\partial V}{\partial S}\right)_P = \frac{\partial^2 H}{\partial S \partial P}$$

$$+\left(\frac{\partial S}{\partial V}\right)_T = +\left(\frac{\partial P}{\partial T}\right)_V = -\frac{\partial^2 F}{\partial T \partial V}$$

$$-\left(\frac{\partial S}{\partial P}\right)_T = +\left(\frac{\partial V}{\partial T}\right)_P = \frac{\partial^2 G}{\partial T \partial P}$$

Useful to check for errors in experiments or calculations

Replace P and V with σ and ε



http://upload.wikimedia.org/wikipedia/commons/0/09/Thermodynamic_map.svg

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INTERNATIONAL TABLES Physical properties of crystals

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International Tables for Crystallography
Volume D: Physical properties of crystals

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Edited by A. Authier

Contents

The properties of solids

$$H = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_A \frac{\hbar^2}{2m_A}\nabla_A^2 - \sum_{i,A}\frac{Z_A e^2}{4\pi\varepsilon_0 r_{iA}} + \sum_{i<j}\frac{e^2}{4\pi\varepsilon_0 r_{ij}} + \sum_{A<B}\frac{Z_A Z_B e^2}{4\pi\varepsilon_0 r_{AB}}$$

electronic band structure E vs. k

structure
bond potentials

phonon band structure ω vs. k

density of states

density of states

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

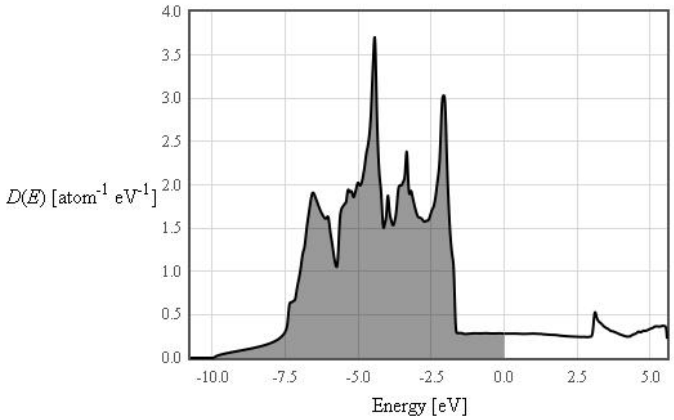
Boltzmann transport

optical
absorption

optical properties

Calculating free energies

Electronic component

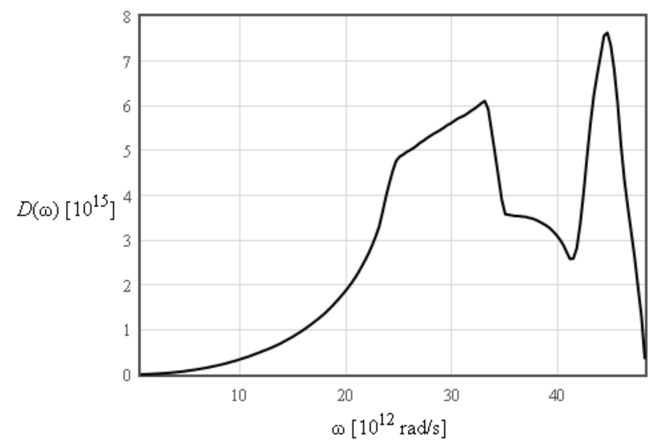


$$n = \int_{-\infty}^{\infty} \frac{D(E)}{1 + \exp\left(\frac{E-\mu}{k_B T}\right)} dE$$

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

Phonon component

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



Groups

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

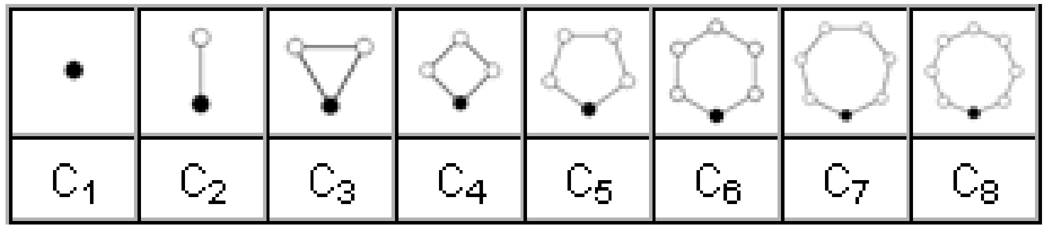
$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & \sin\alpha \\ 0 & -\sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Symmetries can be represented by matrices.
All such matrices that bring the crystal into itself form the group of the crystal.

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

32 point groups (one point remains fixed during transformation)
230 space groups

Cyclic groups



C_2

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

C_4

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

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

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

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, $LaTaO_3$

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

Pyroelectrics have a spontaneous polarization. If it can be reversed by an electric field they are called Ferroelectrics ($BaTiO_3$)

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

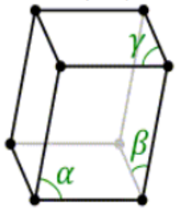
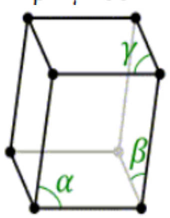
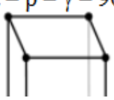
$$U\vec{P} = \chi U\vec{E} \qquad U^{-1}U\vec{P} = U^{-1}\chi U\vec{E} \qquad \chi = U^{-1}\chi U$$

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

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

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

The 32 Crystal Classes

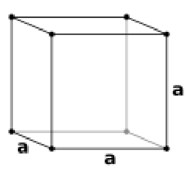
Crystal system	Crystal Class	International symbol	Schoenflies symbol	Space groups	2-fold axes	3-fold axes	4-fold axes	6-fold axes	mirror planes	inversion	Examples	Number of symmetry elements
Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$ 	triclinic-pedial	1	C_1	1: P1	-	-	-	-	-	n		1
	triclinic-pinacoidal	$\bar{1}$	$S_2 = C_i$	2: $P\bar{1}$	-	-	-	-	-	y		2
Monoclinic $a \neq b \neq c$ $\alpha \neq 90°$, $\beta = \gamma = 90°$ 	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 $a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$ 	orthorhombic-disphenoidal	222	$V = D_2$	16: P222, 17: $P222_1$, 18: $P2_12_12$, 19: $P2_12_12_1$, 20: $C222_1$, 21: C222, 22: F222, 23: I222, 24: $I2_12_12_1$	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

Cubic



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

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

Material	ρ (Ω•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]	$2.5e\times10^{-6}$ to 5.0×10^{-6} //basal plane 3.0×10^{-3} ⊥basal plane	2 to 3×10^{5} //basal plane 3.3×10^{2} ⊥basal plane		[17]
Carbon (diamond)[note 8]	1×10^{12}	$\sim10^{-13}$		[18]
Germanium[note 8]	4.6×10^{-1}	2.17	−0.048	[7][8]
Sea water[note 9]	2×10^{-1}	4.8		[19]
Drinking water[note 10]	2×10^{1} to 2×10^{3}	5×10^{-4} to 5×10^{-2}		[citation needed]

WIKIMEDIA

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Rutile

From Wikipedia, the free encyclopedia

```
_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
```

re known:

al mineral of pseudo-octahedral habit

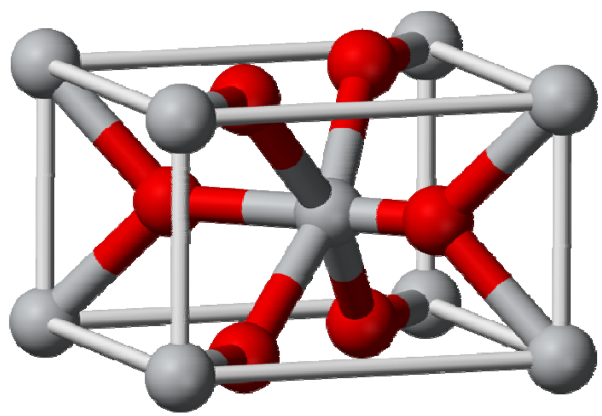
own crystal, and also exhibits a

it is useful for the manufacture of certain

avelengths up to about 4.5μm.

d tantalum. Rutile derives its name from

imens when viewed by transmitted light.



ı high-temperature and high-pressure

s.

able polymorph of TiO_2 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

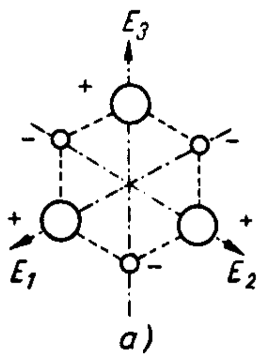
$$g_{36} \rightarrow g_{312}$$

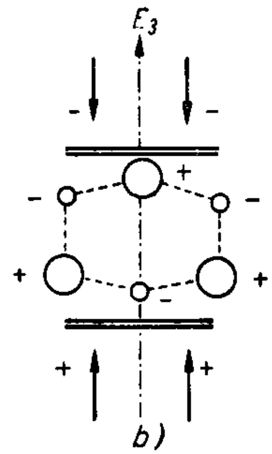
rank 4

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

Piezoelectricity

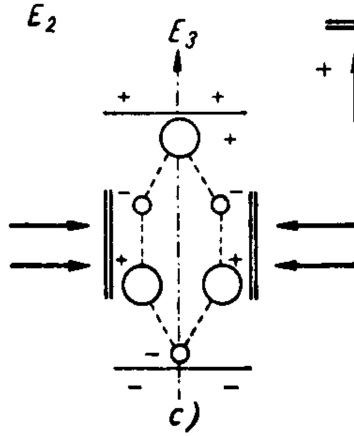
average position
+ is
average position -





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

average position
+ not
average position -

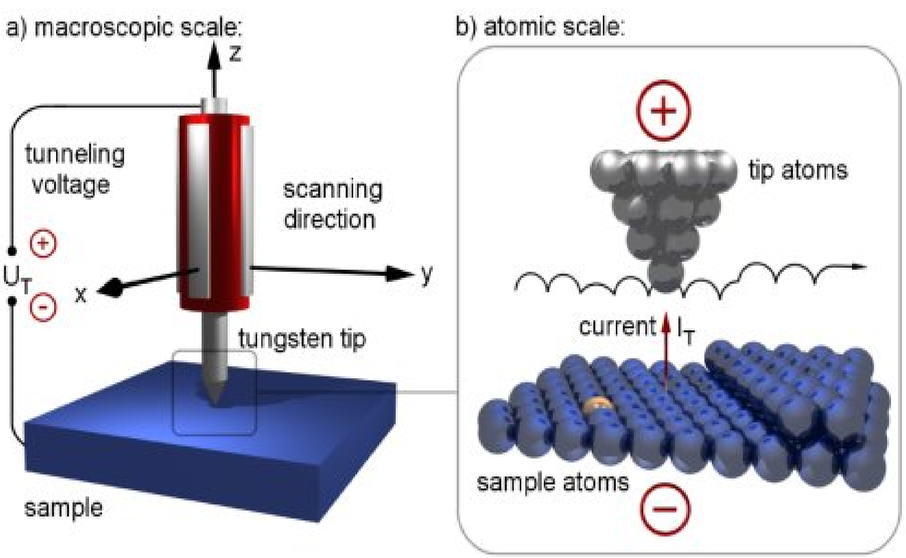


$$\frac{\partial P_k}{\partial \sigma_{ij}} = -\left(\frac{\partial^2 G}{\partial E_k \partial \sigma_{ij}}\right) = d_{ijk}$$

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 ($Pb[Zr_xTi_{1-x}]O_3$ $0<x<1$)
—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)
$Ba_2NaNb_5O_5$
$Pb_2KNb_5O_{15}$

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

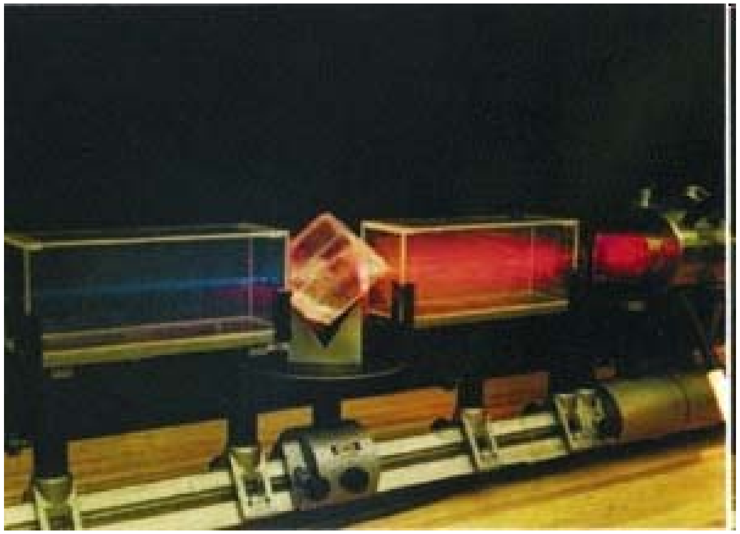
Period doubling crystals

no inversion symmetry

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

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

$$\cos^2(\omega t) = \tfrac{1}{2}\left(1 + \cos(2\omega t)\right)$$

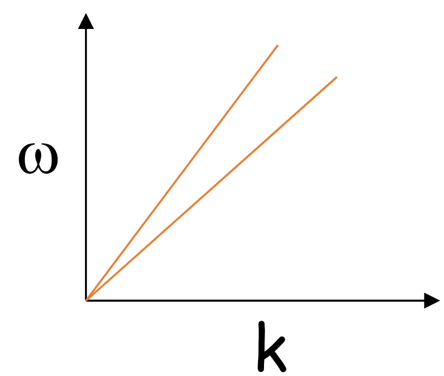


806 nm light : lithium iodate ($LiIO_3$)
860 nm light : potassium niobate ($KNbO_3$)
980 nm light : $KNbO_3$
1064 nm light : monopotassium phosphate (KH_2PO_4, KDP), lithium triborate (LBO).
1300 nm light : gallium selenide (GaSe)
1319 nm light : $KNbO_3$, BBO, KDP, lithium niobate ($LiNbO_3$), $LiIO_3$

Birefringence (Doppelbrechung)

Calcite

Two indices of refraction



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