Symmetries, Crystal physics

Crystal Physics

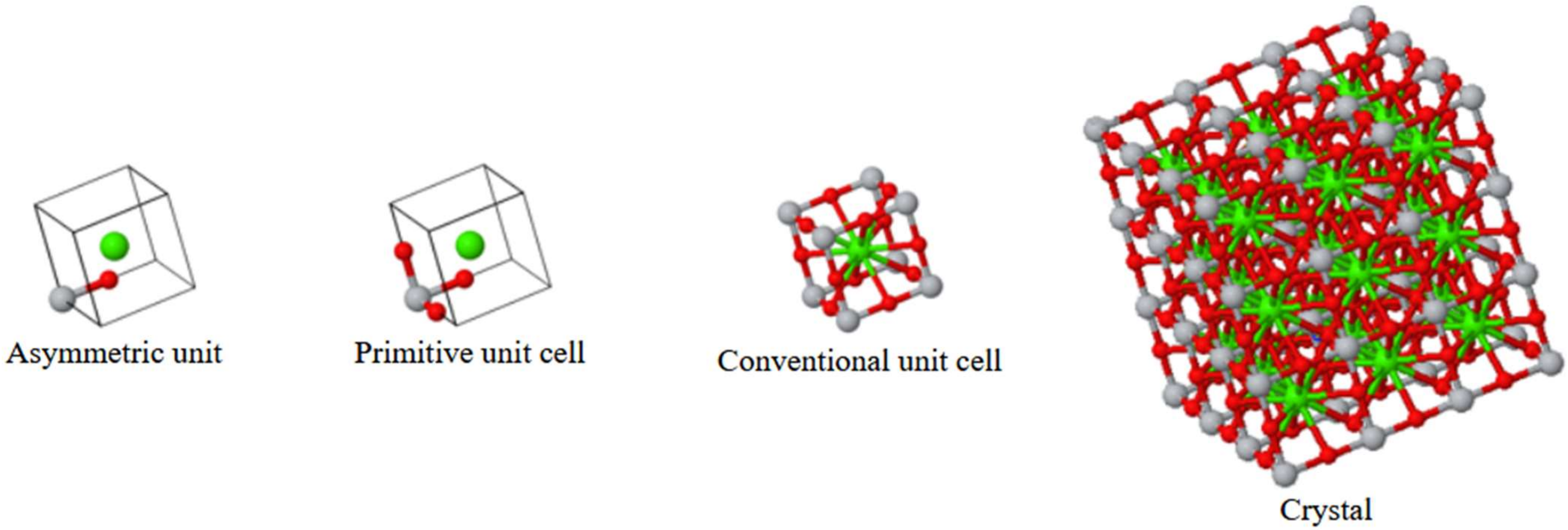
Crystal physics explains what effects the symmetries of the crystal have on observable quantities.

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

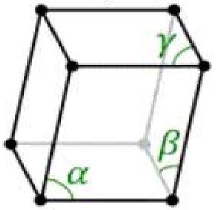
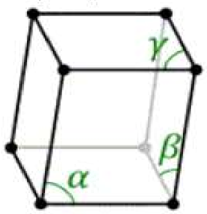
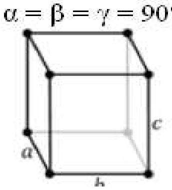
International Tables for Crystallography
http://it.iucr.org/

Kittel chapter 3: elastic strain

Asymmetric unit



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	N sy el
Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$ 	triclinic-pedial	1	C_1	1	-	-	-	-	-	n		
	triclinic-pinacoidal	$\bar{1}$	$S_2 = C_i$	2	-	-	-	-	-	y		
Monoclinic $a \neq b \neq c$ $\alpha \neq 90°$, $\beta = \gamma = 90°$ 	monoclinic-sphenoidal	2	C_2	3-5	1	-	-	-	-	n		
	monoclinic-domatic	m	$C_{1h} = C_s$	6-9	-	-	-	-	1	n		
	monoclinic-prismatic	$2/m$	C_{2h}	10-15	1	-	-	-	1	y		
Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$ 	orthorhombic-disphenoidal	222	$V = D_2$	16-24	3	-	-	-	-	n		
	orthorhombic-pyramidal	$mm2$	C_{2v}	25-46	1	-	-	-	2	n		
											47: $YBa_2Cu_3O_{7-x}$	

http://lamp.tu-graz.ac.at/~hadley/ss2/crystalphysics/crystalclasses/crystalclasses.html

Sodalite

From Wikipedia, the free encyclopedia

Sodalite is a rich royal blue mineral widely enjoyed as an ornamental gemstone. Although massive sodalite samples are opaque, crystals are usually transparent to translucent. Sodalite is a member of the sodalite group with hauyne, nosean, lazurite and tugtupite.

Discovered in 1811 in the Ilimaussaq intrusive complex in Greenland, sodalite did not become important as an ornamental stone until 1891 when vast deposits of fine material were discovered in Ontario, Canada.

Contents [hide]

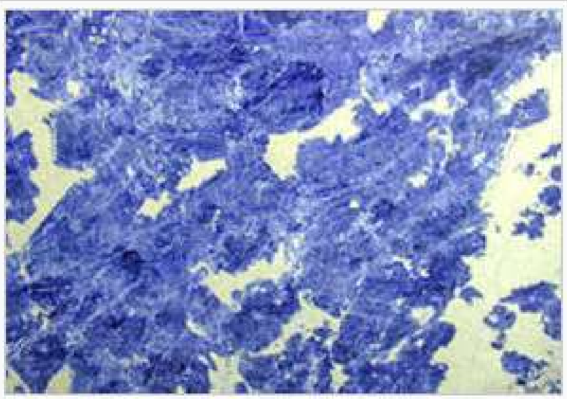
Sodalite	

A sample of sodalite

General	
Category	Tectosilicates without zeolitic H_2O
Formula (repeating unit)	$Na_8(Al_6Si_6O_{24})Cl_2$
Strunz classification	09.FB.10
Crystal symmetry	Isometric hextetrahedral H-M symbol: $\bar{4}3m$ Space group: $P\bar{4}3n$
Unit cell	a = 8.876(6) Å; Z = 1

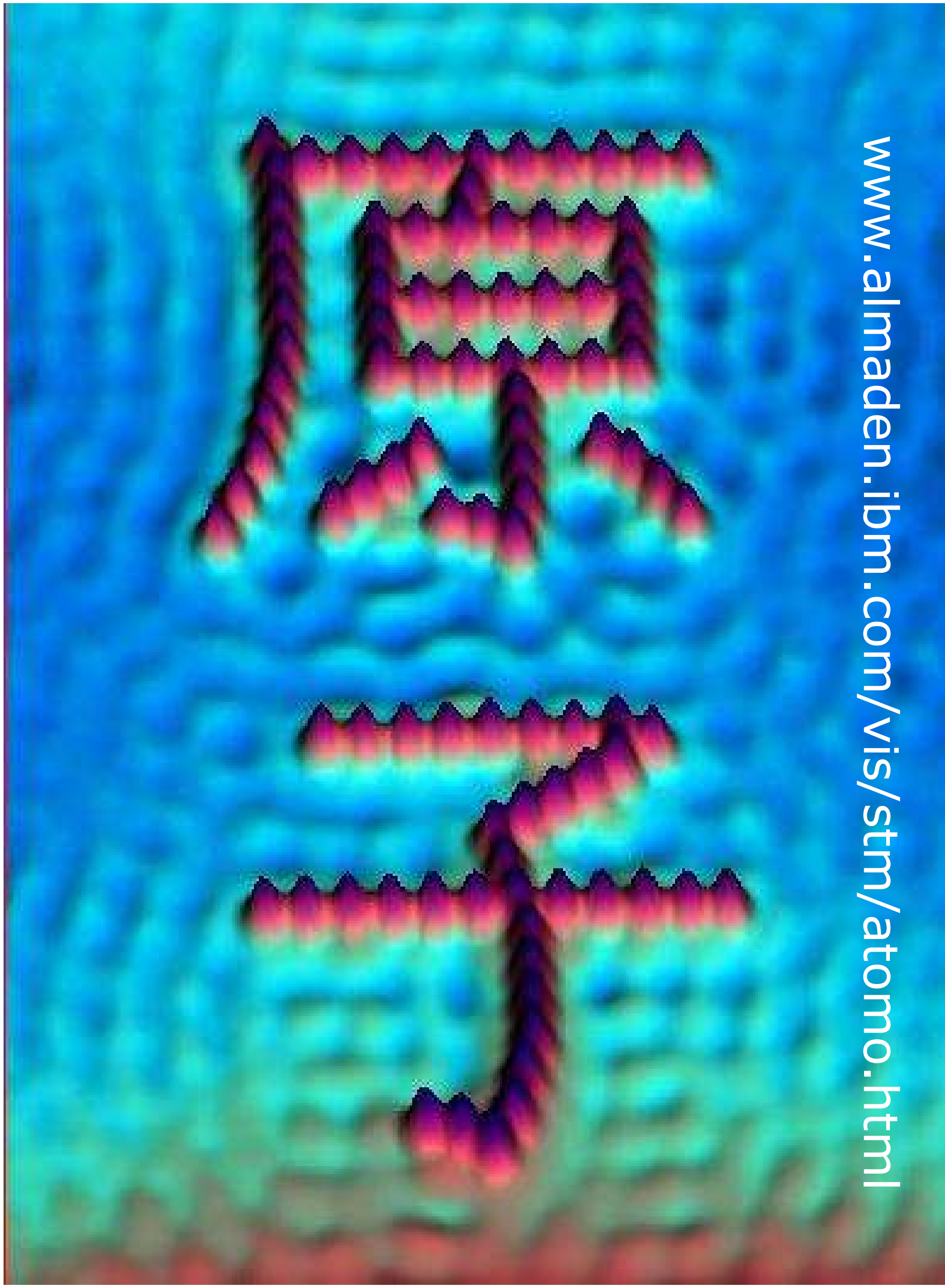
Identification

Properties [edit]



A sample of **sodalite**-carbonate pegmatite from Bolivia, with a polished rock

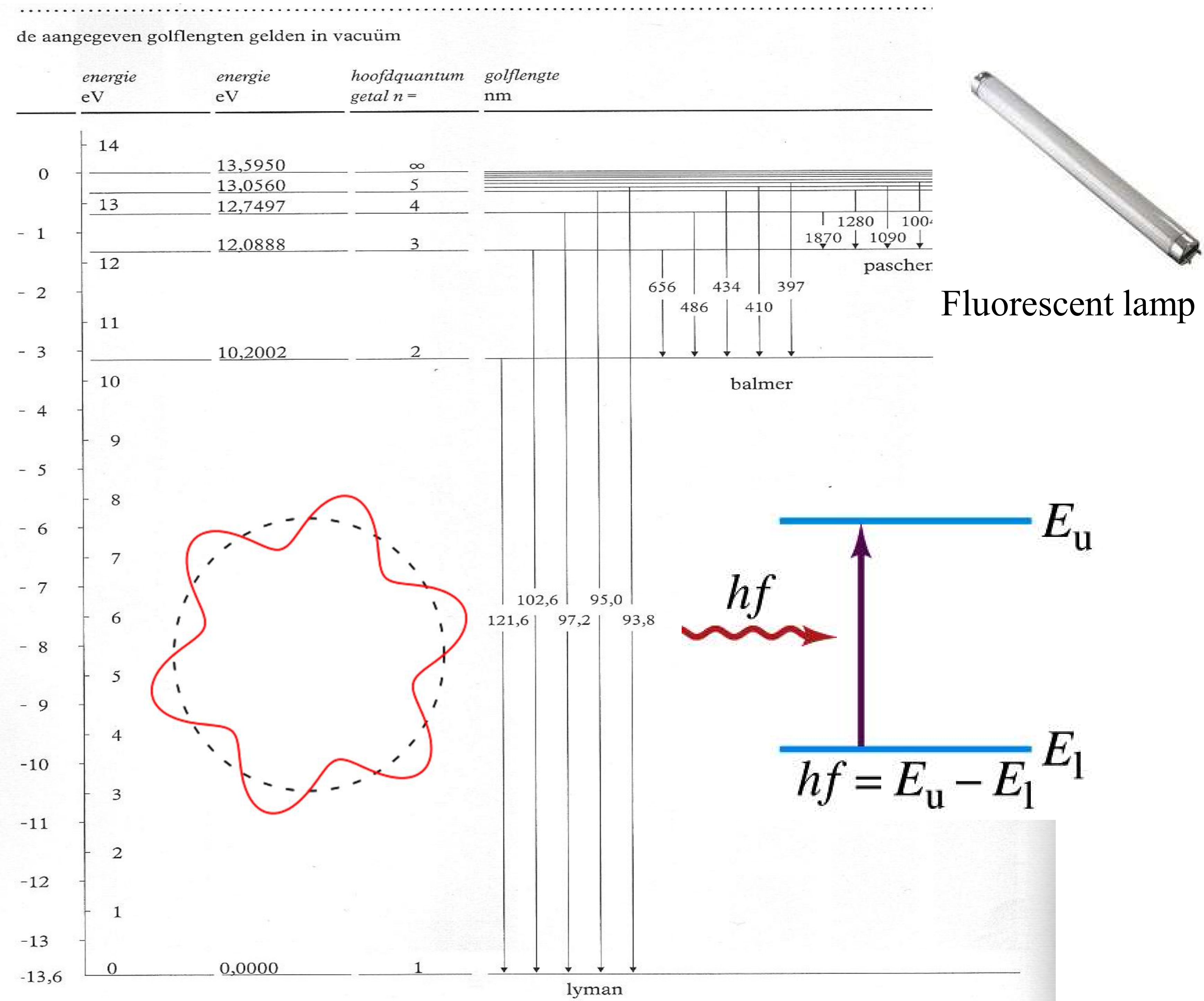
A light, relatively hard yet fragile mineral, sodalite is named after its sodium content; in mineralogy it may be classed as a feldspathoid. Well known for its blue color, sodalite may also be grey, yellow, green, or pink and is often mottled with white veins or patches. The more uniformly blue material is used in jewellery, where it is fashioned into cabochons and beads. Lesser material is more often seen as facing or inlay in



Quantum Mechanics

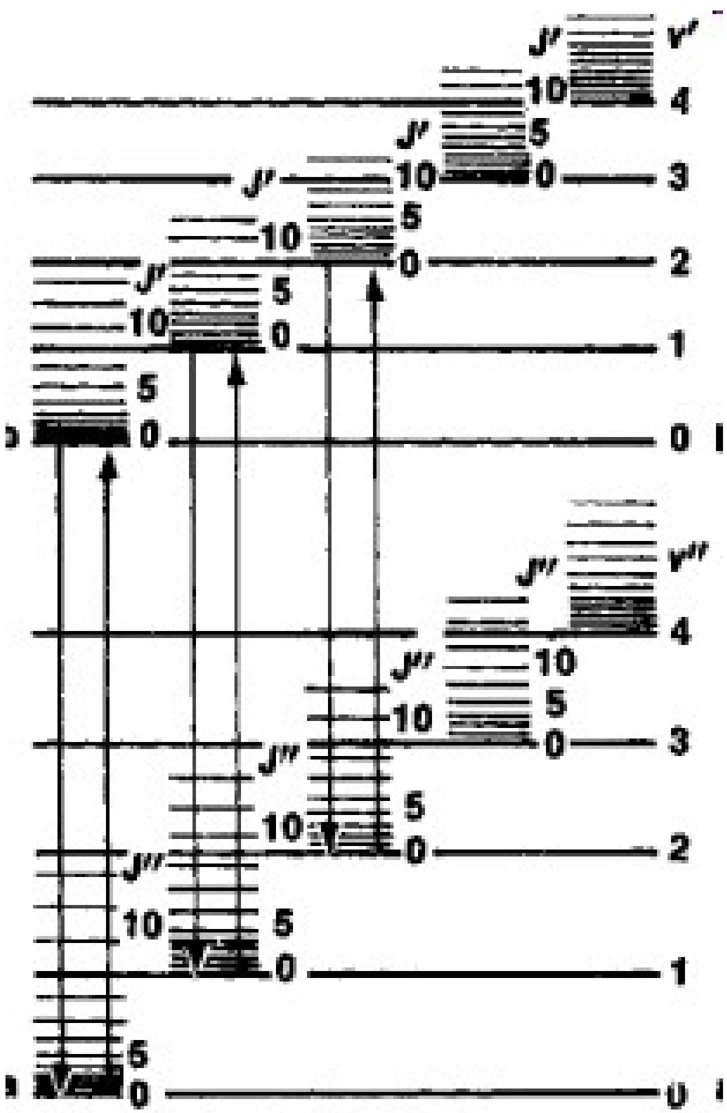
Everything moves like a wave but exchanges energy and momentum like a particle.

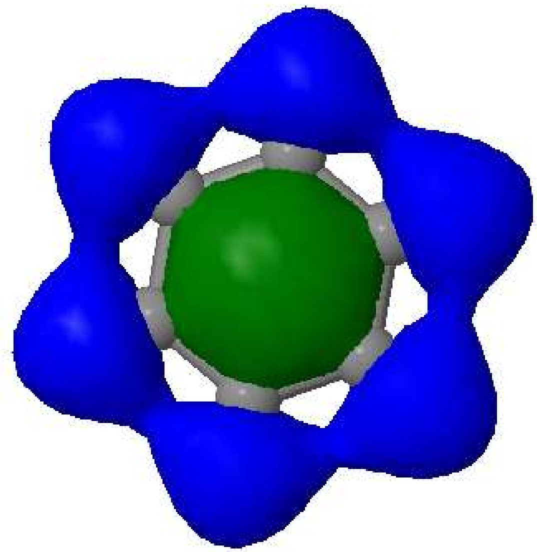
Everything moves like a wave but exchanges energy and momentum like a particle.

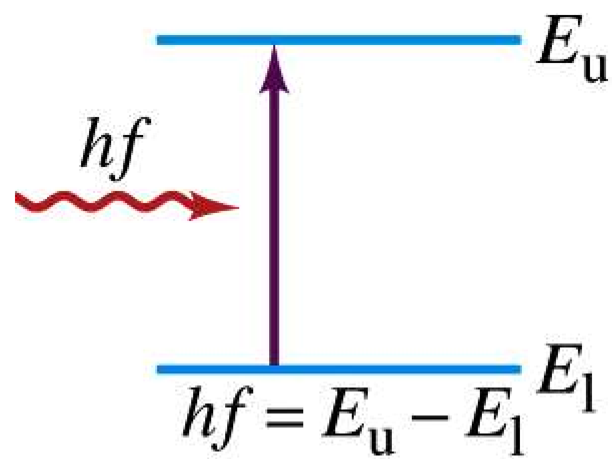


Fluorescent lamp

Molecular energy levels







Gibbs free energy

$$G(T,\sigma_{ij},E_k,M_l)$$

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

$$\left(\frac{\partial G}{\partial \sigma_{ij}}\right) = -\varepsilon_{ij} \qquad \left(\frac{\partial G}{\partial E_k}\right) = -P_k$$

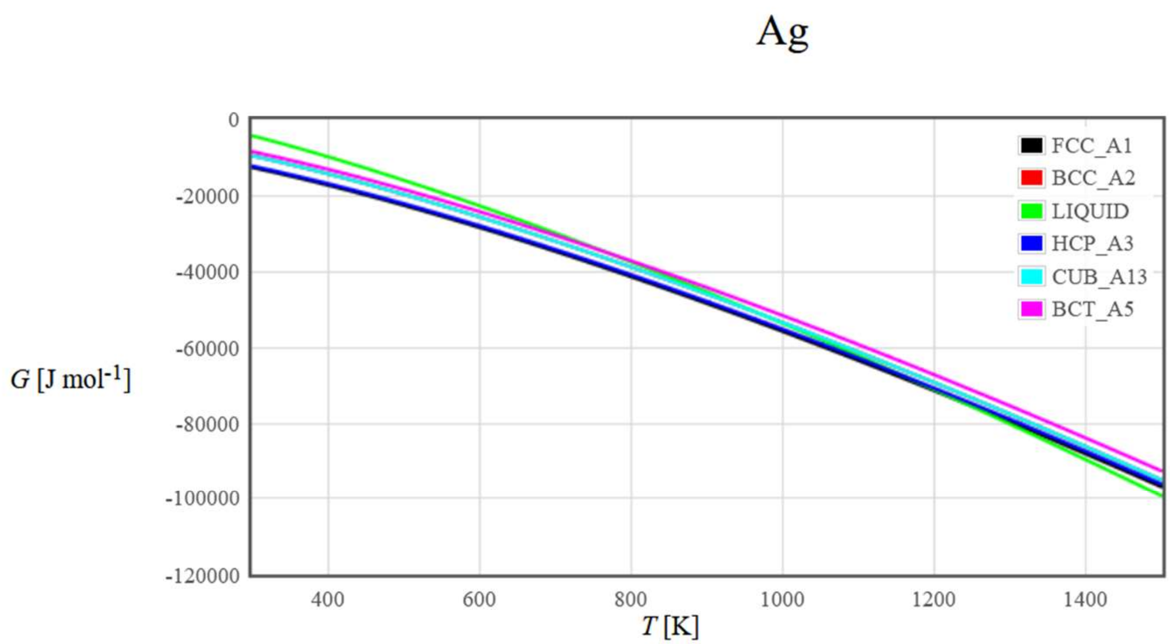
$$\left(\frac{\partial G}{\partial H_l}\right) = -M_l \qquad \left(\frac{\partial G}{\partial T}\right) = -S$$

SGTE thermodynamic data

The Scientific Group Thermodata Europe SGTE maintains thermodynamic databanks for inorganic and metallurgical systems. Data from their 'pure element database' is plotted below.

Typically, experiments are performed at constant pressure p, temperature T, and number N. Under these conditions, the system will go to the minimum of the Gibbs energy $G = U + pV - TS$. Here U is the internal energy, V is the volume, and S is the entropy. The top plot is the Gibbs energy per mole.

Ag	Al	Am	As
Au	B	Ba	Be
Bi	C	Ca	Cd
Ce	Co	Cr	Cs
Cu	Dy	Er	Eu
Fe	Ga	Gd	Ge
Hf	Hg	Ho	In
Ir	K	La	Li
Lu	Mg	Mn	Mo
N	Na	Nb	Nd
Ni	Np	O	Os
P	Pa	Pb	Pd
Pr	Pt	Pu	Rb
Re	Rh	Ru	S
Sb	Sc	Se	Si
Sm	Sn	Sr	Ta
Tb	Tc	Te	Th
Ti	Tl	Tm	U
V	W	Y	Yb
Zn	Zr		



Since the Gibbs energies of the different phases fall almost on top of each other, it is convenient to plot them relative to the phase that has the lowest Gibbs energy at low temperature.

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

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

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

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

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.

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

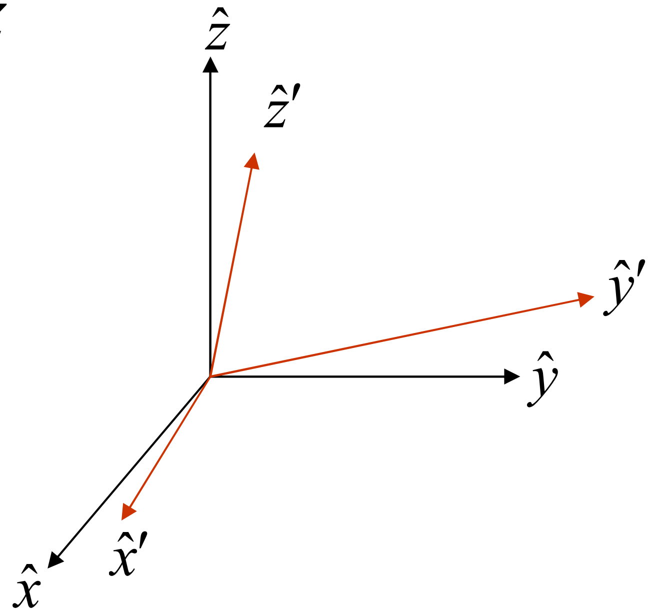
Strain

A distortion of a material is described by the strain matrix

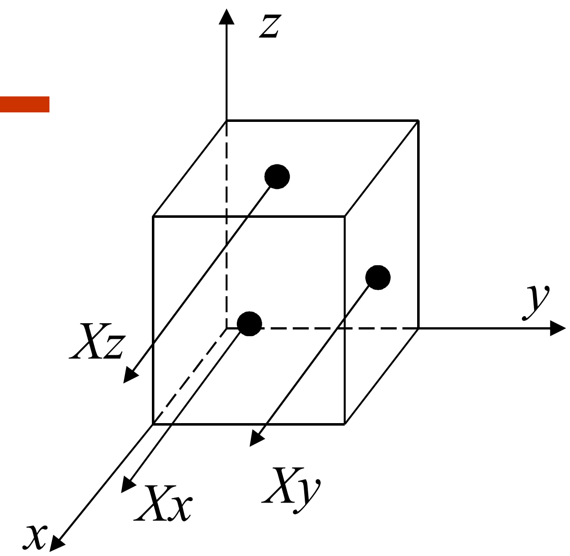
$$x' = (1+\varepsilon_{xx})\hat{x} + \varepsilon_{xy}\hat{y} + \varepsilon_{xz}\hat{z}$$

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

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



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.

$$\varepsilon_{xx} = s_{xxxx}\sigma_{xx} + s_{xxxy}\sigma_{xy} + s_{xxxz}\sigma_{xz} + s_{xxyx}\sigma_{yx} + s_{xxyy}\sigma_{yy}$$
$$+ s_{xxyz}\sigma_{yz} + s_{xxzx}\sigma_{zx} + s_{xxzy}\sigma_{zy} + s_{xxzz}\sigma_{zz}$$

Tensors

Rank 2 tensors couple two vectors:
Electrical conductivity, thermal conductivity, electric susceptibility, magnetic susceptibility, Peltier effect (heat current due to electrical current), Seebeck effect (Electric field due to thermal gradient)

Rank 3 tensors couple a vector to a matrix:
Piezoelectricity, piezomagnetism

Rank 4 tensors couple two matrices:
Stiffness, compliance, piezoconductivity

Point Groups

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

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

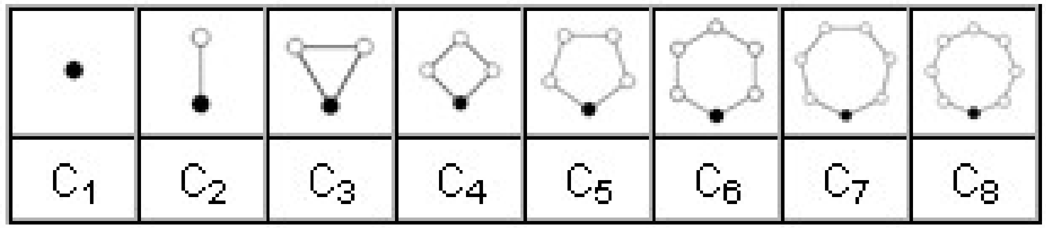
Symmetries can be represented by matrices.
All such matrices that bring the crystal into itself form the group of the crystal.

$$\mathrm{AB} \in \mathrm{G} \text{ for } \mathrm{A, B} \in \mathbf{G}$$

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

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,

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

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

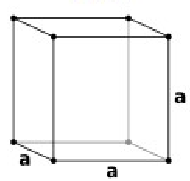
Cubic crystals

All second rank tensors of cubic crystals reduce to constants

Electrical conductivity, thermal conductivity, electric susceptibility, magnetic susceptibility, Peltier effect (heat current due to electrical current), Seebeck effect (Electric field due to thermal gradient)

216: ZnS, GaAs, GaP, InAs, SiC
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



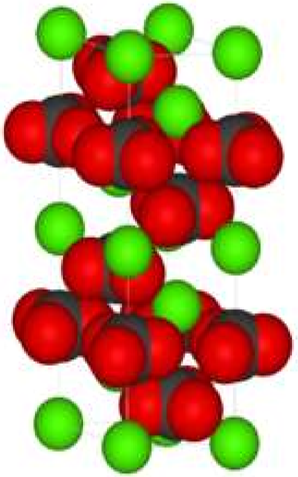
23	T	195-199		12
$m3$	T_h	200-206		24
432	O	207-214		24
$\bar{4}3m$	T_d	215-220	216: Zincblende, ZnS, GaAs, GaP, InAs, SiC	24
$m3m$	O_h	221-230	221: CsCl, cubic perovskite 225: fcc, Al, Cu, Ni, Ag, Pt, Au, Pb, γ-Fe, NaCl 227: diamond, C, Si,	48

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

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]

Birefringence

Calcite

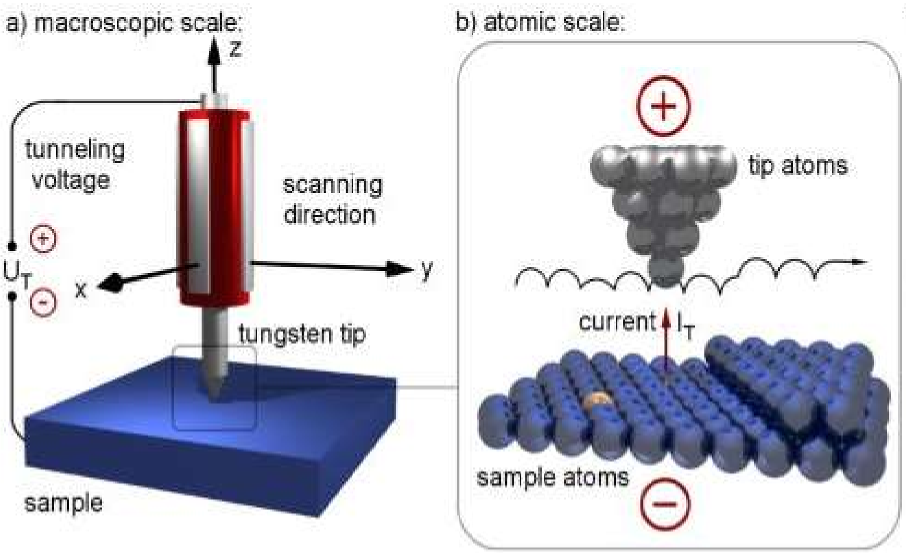


name	international	Schoenflies	examples
rhombohedral holohedral	$\bar{3}m$	D_{3d}	calcite, corundum, hematite
rhombohedral hemimorphic	$3m$	C_{3v}	tourmaline, alunite
rhombohedral tetartohedral	$\bar{3}$	S_6	dolomite, ilmenite
trapezohedral	32	D_3	quartz, cinnabar
rhombohedral tetartohedral	3	C_3	none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

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

Electrostriction

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

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

piezoelectricity

Electrostriction

Nonlinear optics

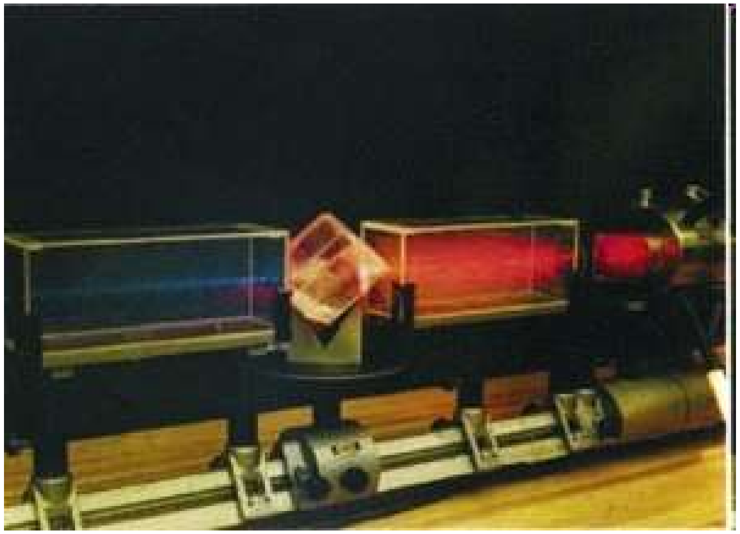
Period doubling crystals

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 ($LiNbO_3$), $LiIO_3$

Symmetric Tensors

$$\chi_{ij}^{E} = \frac{\partial P_i}{\partial E_j} = -\frac{\partial^2 G}{\partial E_i \partial E_j} = \frac{\partial P_j}{\partial E_i} = \chi_{ji}^{E}$$

$$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{12} & g_{22} & g_{23} \\ g_{13} & g_{23} & g_{33} \end{bmatrix}$$

Tensor notation

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

$$
\begin{array}{lll}
1\,1 \to 1 & 1\,2 \to 6 & 1\,3 \to 5 \\
 & 2\,2 \to 2 & 2\,3 \to 4 \\
 & & 3\,3 \to 3
\end{array}
$$

rank 3

$$g_{36} \to g_{312}$$

rank 4

$$g_{14} \to g_{1123}$$

rank 2 symmetric tensors[2]	rank 2 asymmetric tensors	rank 3 tensors[3]	rank 4 tensors
$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{12} & g_{22} & g_{23} \\ g_{13} & g_{23} & g_{33} \end{bmatrix}$	$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix}$	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & g_{14} & g_{15} & g_{16} \\ g_{21} & g_{22} & g_{23} & g_{24} & g_{25} & g_{26} \\ g_{31} & g_{32} & g_{33} & g_{34} & g_{35} & g_{36} \end{bmatrix}$ reduced, symmetric, asymmetric	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & g_{14} & g_{15} & g_{16} \\ g_{21} & g_{22} & g_{23} & g_{24} & g_{25} & g_{26} \\ g_{31} & g_{32} & g_{33} & g_{34} & g_{35} & g_{36} \\ g_{41} & g_{42} & g_{43} & g_{44} & g_{45} & g_{46} \\ g_{51} & g_{52} & g_{53} & g_{54} & g_{55} & g_{56} \\ g_{61} & g_{62} & g_{63} & g_{64} & g_{65} & g_{66} \end{bmatrix}$ reduced, symmetric, asymmetric
	$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ reduced, symmetric, asymmetric	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & g_{14} & g_{15} & g_{16} \\ g_{21} & g_{22} & g_{23} & g_{24} & g_{25} & g_{26} \\ g_{31} & g_{32} & g_{33} & g_{34} & g_{35} & g_{36} \\ g_{41} & g_{42} & g_{43} & g_{44} & g_{45} & g_{46} \\ g_{51} & g_{52} & g_{53} & g_{54} & g_{55} & g_{56} \\ g_{61} & g_{62} & g_{63} & g_{64} & g_{65} & g_{66} \end{bmatrix}$ reduced, symmetric, asymmetric
$\begin{bmatrix} g_{11} & g_{12} & 0 \\ g_{12} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} g_{11} & g_{12} & 0 \\ g_{21} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 & g_{14} & g_{15} & 0 \\ 0 & 0 & 0 & g_{24} & g_{25} & 0 \\ g_{31} & g_{32} & g_{33} & 0 & 0 & g_{36} \end{bmatrix}$ reduced, symmetric, asymmetric	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & 0 & 0 & g_{16} \\ g_{21} & g_{22} & g_{23} & 0 & 0 & g_{26} \\ g_{31} & g_{32} & g_{33} & 0 & 0 & g_{36} \\ 0 & 0 & 0 & g_{44} & g_{45} & 0 \\ 0 & 0 & 0 & g_{54} & g_{55} & 0 \\ g_{61} & g_{62} & g_{63} & 0 & 0 & g_{66} \end{bmatrix}$ reduced, symmetric, asymmetric
	$\begin{bmatrix} g_{11} & g_{12} & 0 \\ g_{21} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & 0 & 0 & g_{16} \\ g_{21} & g_{22} & g_{23} & 0 & 0 & g_{26} \\ 0 & 0 & 0 & g_{34} & g_{35} & 0 \end{bmatrix}$ reduced, symmetric, asymmetric	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & 0 & 0 & g_{16} \\ g_{21} & g_{22} & g_{23} & 0 & 0 & g_{26} \\ g_{31} & g_{32} & g_{33} & 0 & 0 & g_{36} \\ 0 & 0 & 0 & g_{44} & g_{45} & 0 \\ 0 & 0 & 0 & g_{54} & g_{55} & 0 \\ g_{61} & g_{62} & g_{63} & 0 & 0 & g_{66} \end{bmatrix}$ reduced, symmetric, asymmetric
	$\begin{bmatrix} g_{11} & g_{12} & 0 \\ g_{21} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ reduced, symmetric, asymmetric	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & 0 & 0 & g_{16} \\ g_{21} & g_{22} & g_{23} & 0 & 0 & g_{26} \\ g_{31} & g_{32} & g_{33} & 0 & 0 & g_{36} \\ 0 & 0 & 0 & g_{44} & g_{45} & 0 \\ 0 & 0 & 0 & g_{54} & g_{55} & 0 \\ g_{61} & g_{62} & g_{63} & 0 & 0 & g_{66} \end{bmatrix}$ reduced, symmetric, asymmetric
rank 2 symmetric tensors[2]	rank 2 asymmetric tensors	rank 3 tensors[3]	rank 4 tensors
	$\begin{bmatrix} g_{11} & 0 & 0 \\ 0 & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 & g_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & g_{25} & 0 \\ 0 & 0 & 0 & 0 & 0 & g_{36} \end{bmatrix}$ reduced, symmetric, asymmetric	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & 0 & 0 & 0 \\ g_{21} & g_{22} & g_{23} & 0 & 0 & 0 \\ g_{31} & g_{32} & g_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & g_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & g_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & g_{66} \end{bmatrix}$ reduced, symmetric, asymmetric

http://lamp.tu-graz.ac.at/~hadley/ss2/crystalphysics/crystalclasses/crystalclasses.html