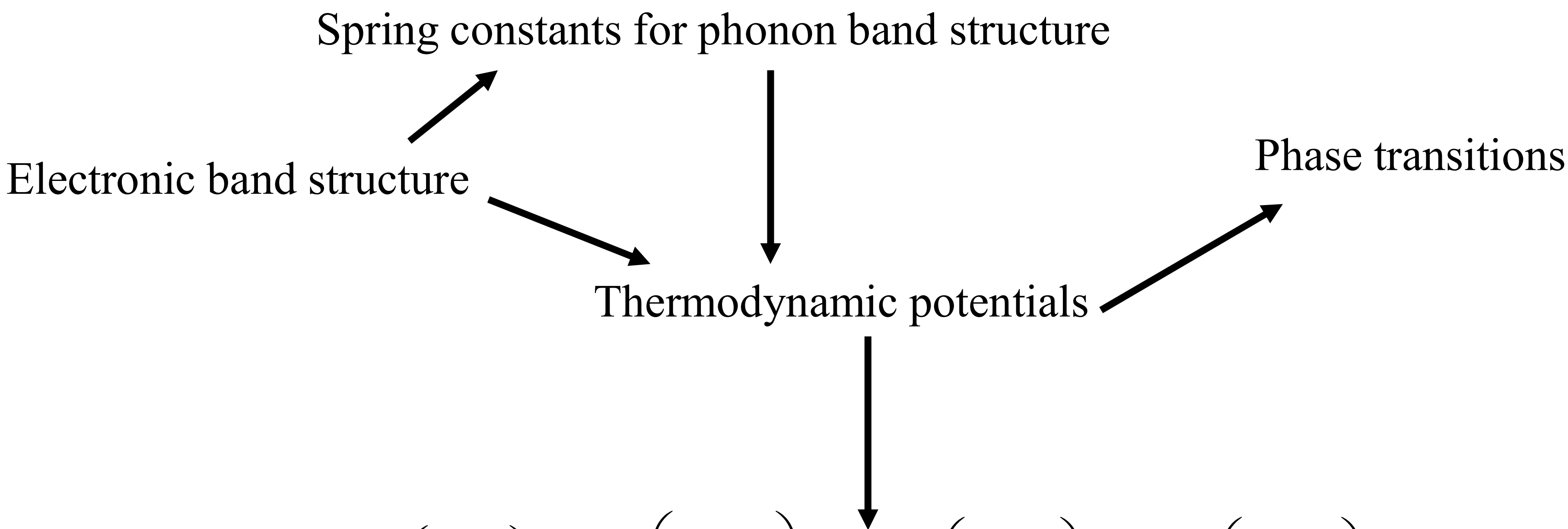
Crystal physics

Thermodynamic properties



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

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

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

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

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

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

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

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

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.

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

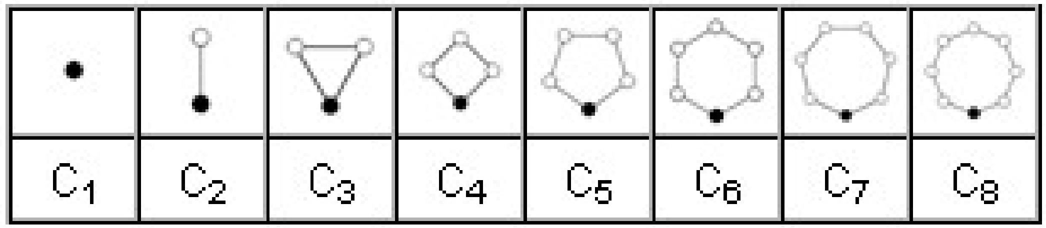
32 point groups (one point remains fixed during transformation)

230 space groups

Space Group	Bravais Lattice
1	Triclinic
2	Triclinic
3	Simple Monoclinic
4	Simple Monoclinic
5	Base-Centered Monoclinic
6	Simple Monoclinic
7	Simple Monoclinic
8	Base-Centered Monoclinic
9	Base-Centered Monoclinic
10	Simple Monoclinic
11	Simple Monoclinic
12	Base-Centered Monoclinic
13	Simple Monoclinic
14	Simple Monoclinic
15	Base-Centered Monoclinic
16	Simple Orthorhombic
17	Simple Orthorhombic
18	Simple Orthorhombic
19	Simple Orthorhombic
20	Base-Centered Orthorhombic
21	Base-Centered Orthorhombic
22	Face-Centered Orthorhombic
23	Body-Centered Orthorhombic
24	Body-Centered Orthorhombic
25	Simple Orthorhombic
26	Simple Orthorhombic
27	Simple Orthorhombic

http://lampx.tugraz.at/~hadley/ss1/crystalstructure/sg2bravais.html

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 ΔT = 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

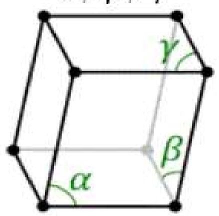
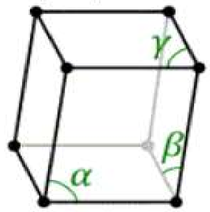
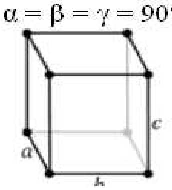
$$U\vec{P} = \chi U\vec{E} \qquad U^{-1}U\vec{P} = U^{-1}\chi U\vec{E} \qquad \chi = U^{-1}\chi U$$

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

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

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

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: $YBa_2Cu_3O_{7-x}$	

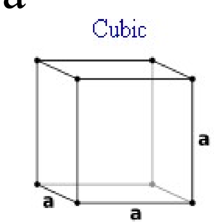
http://lamp.tu-graz.ac.at/~hadley/ss2/crystalphysics/crystalclasses/crystalclasses.html

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



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

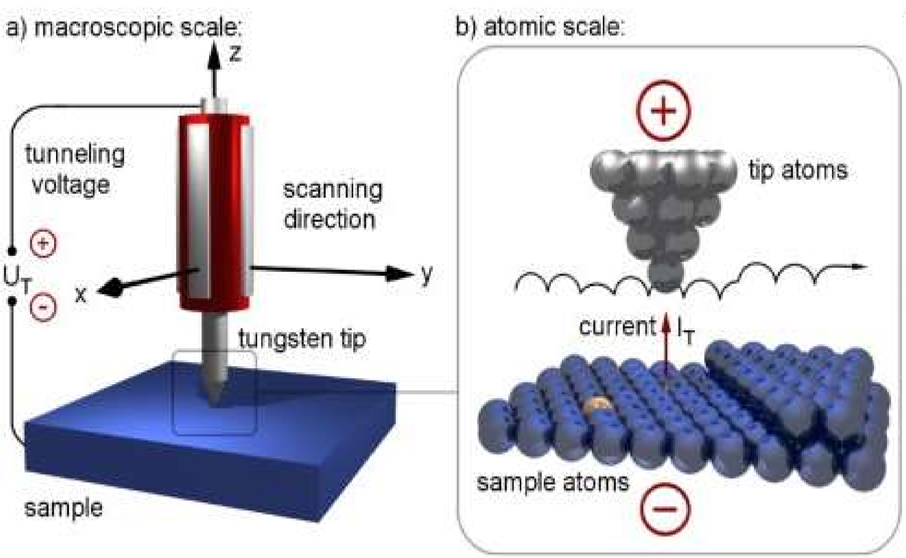
$$\begin{bmatrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{11} \end{bmatrix}$$

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]

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

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.

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

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

$$3\,3 \rightarrow 3$$

rank 3

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

rank 4

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

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

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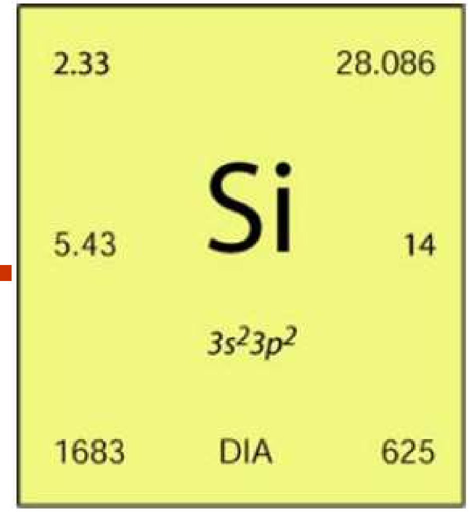
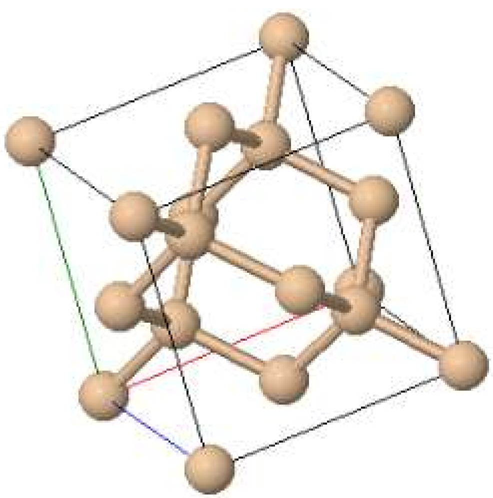
Semiconductors

Silicon



- Important semiconducting material
- 2nd most common element on earths crust (rocks, sand, glass, concrete)
- Often doped with other elements
- Oxide SiO_2 is a good insulator



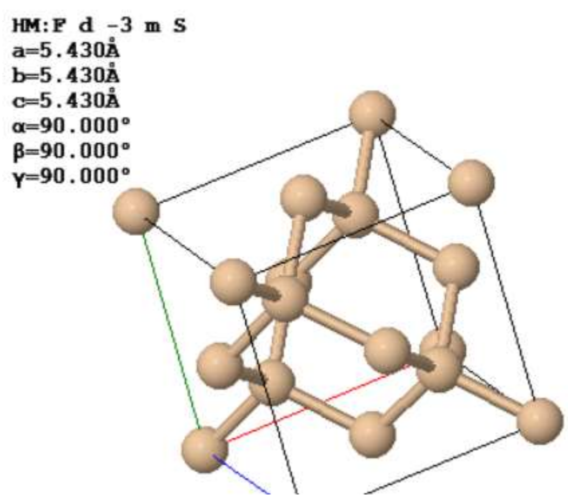
silicon crystal = diamond crystal structure

Silicon

Silicon is the second most common element in the earth's crust and an important semiconducting material.

Structural properties

Crystal structure: Diamond
Bravais lattice: face centered cubic
Space group: 227 (F d -3 m), Strukturbericht: A4, Pearson symbol: cF8
Point group: m3m (O_h) six 2-fold rotations, four 3-fold rotations, three 4-fold rotations, nine mirror planes, inversion
Lattice constant: $a = 0.543$ nm
Atomic weight 28.09
Atomic density $n_{atoms} = 4.995 \times 10^{22}$ 1/cm³
Density $\rho = 2.33$ g/cm³
Density of surface atoms
(100) 6.78×10^{14} 1/cm²
(110) 9.59×10^{14} 1/cm²
(111) 7.83×10^{14} 1/cm²

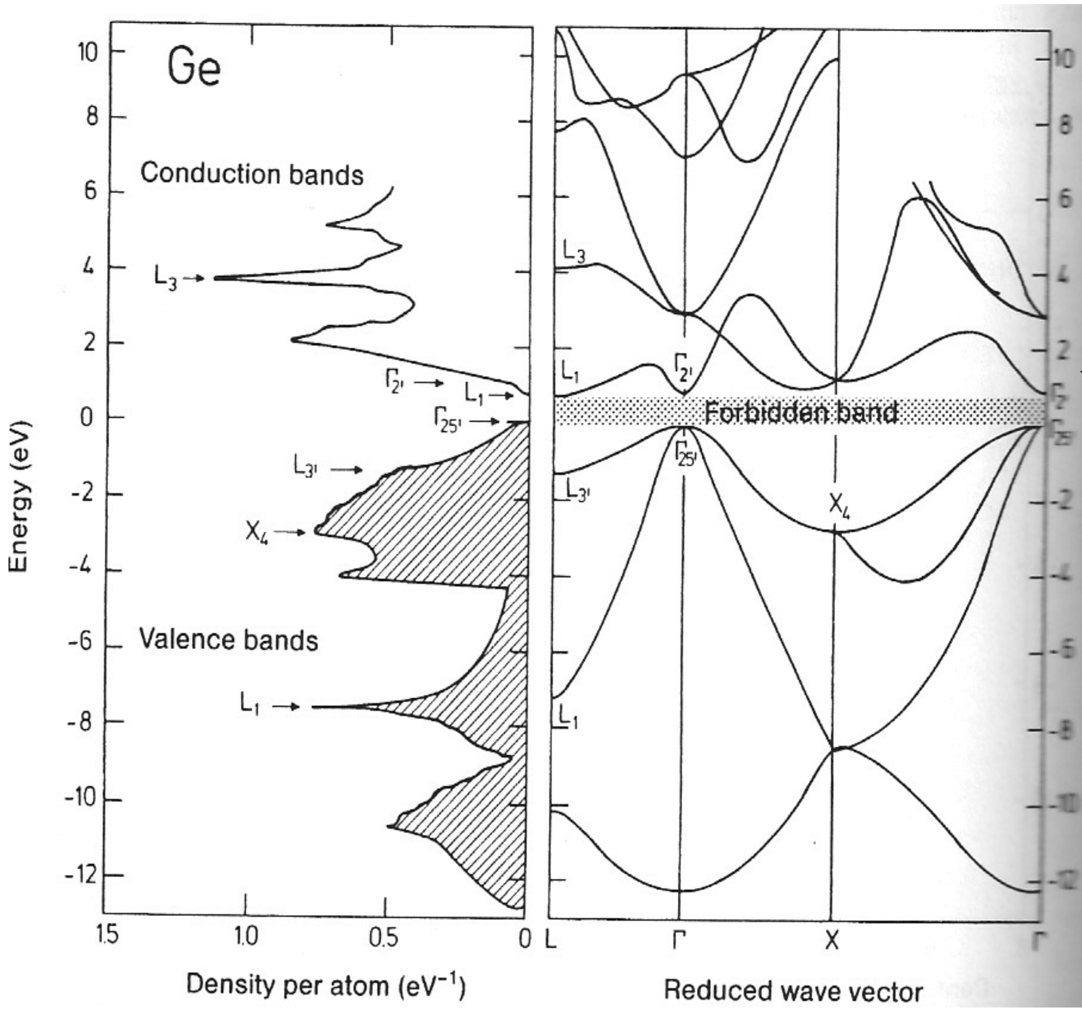


Conventional unit cell | Primitive unit cell | Asymmetric unit
2 x 2 x 2 | 3 x 3 x 3 | 5 x 5 x 5
Ball and Stick | Spacefill

H: 1 K: 0 L: 0
show HKL plane | hide HKL plane
draw atoms in HKL plane
Thickness of HKL planes:

The conventional unit cell is a cube with sides of 0.543 nm. There are 8 atoms atoms in the conventional unit cell. (The

Semiconductors



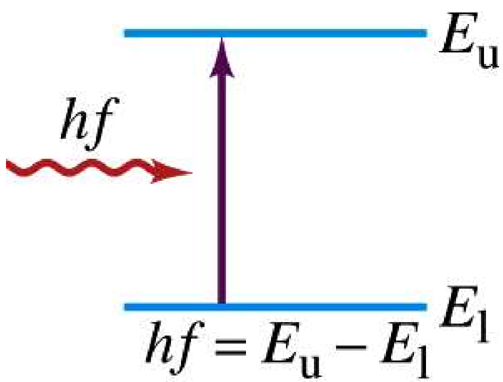
Conduction band

Valence band

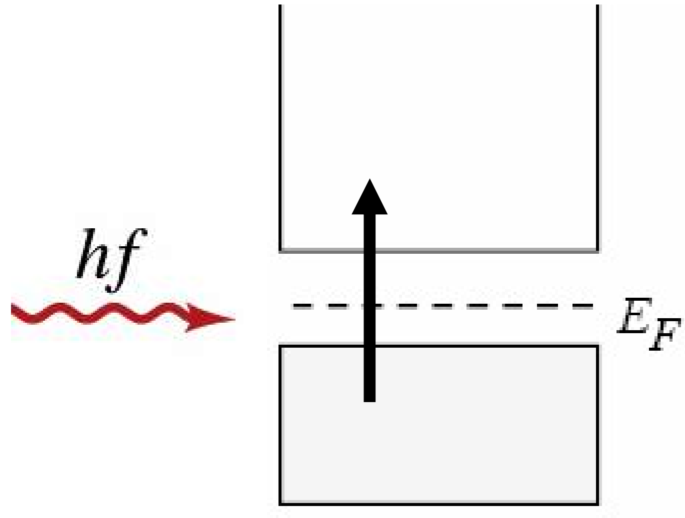
$$n = \int_{-\infty}^{\infty} D(E) f(E) dE$$

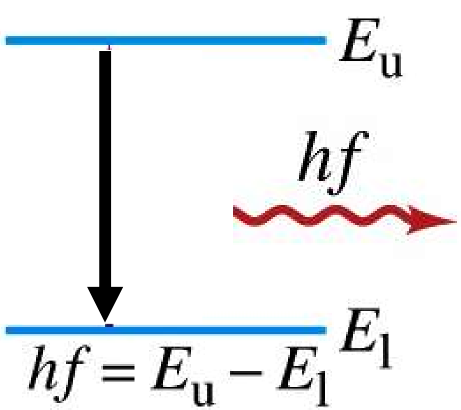
From Ibach & Lueth

Absorption and emission of photons

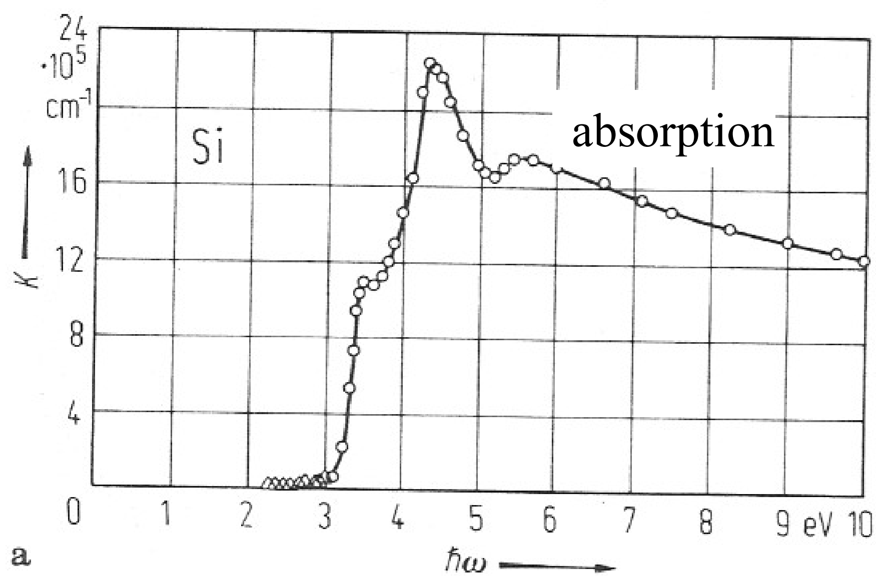


absorption

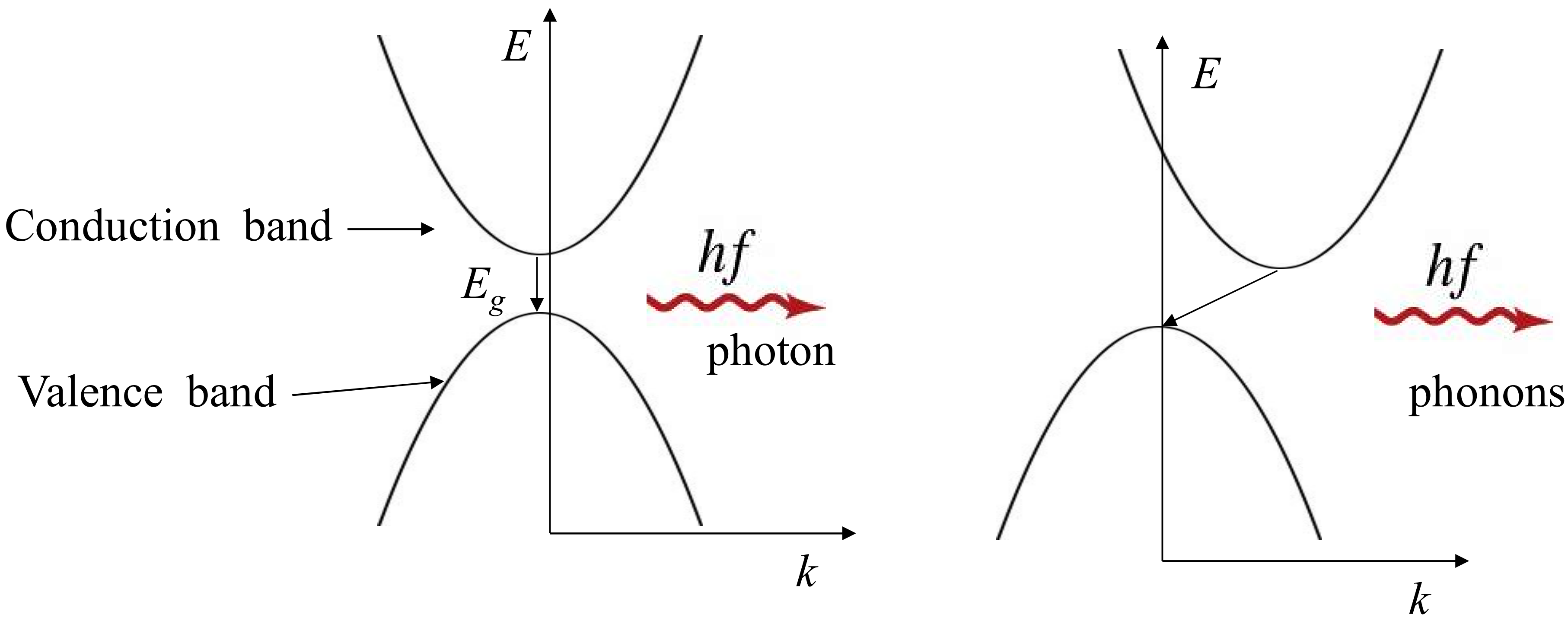




emission



Direct and indirect band gaps

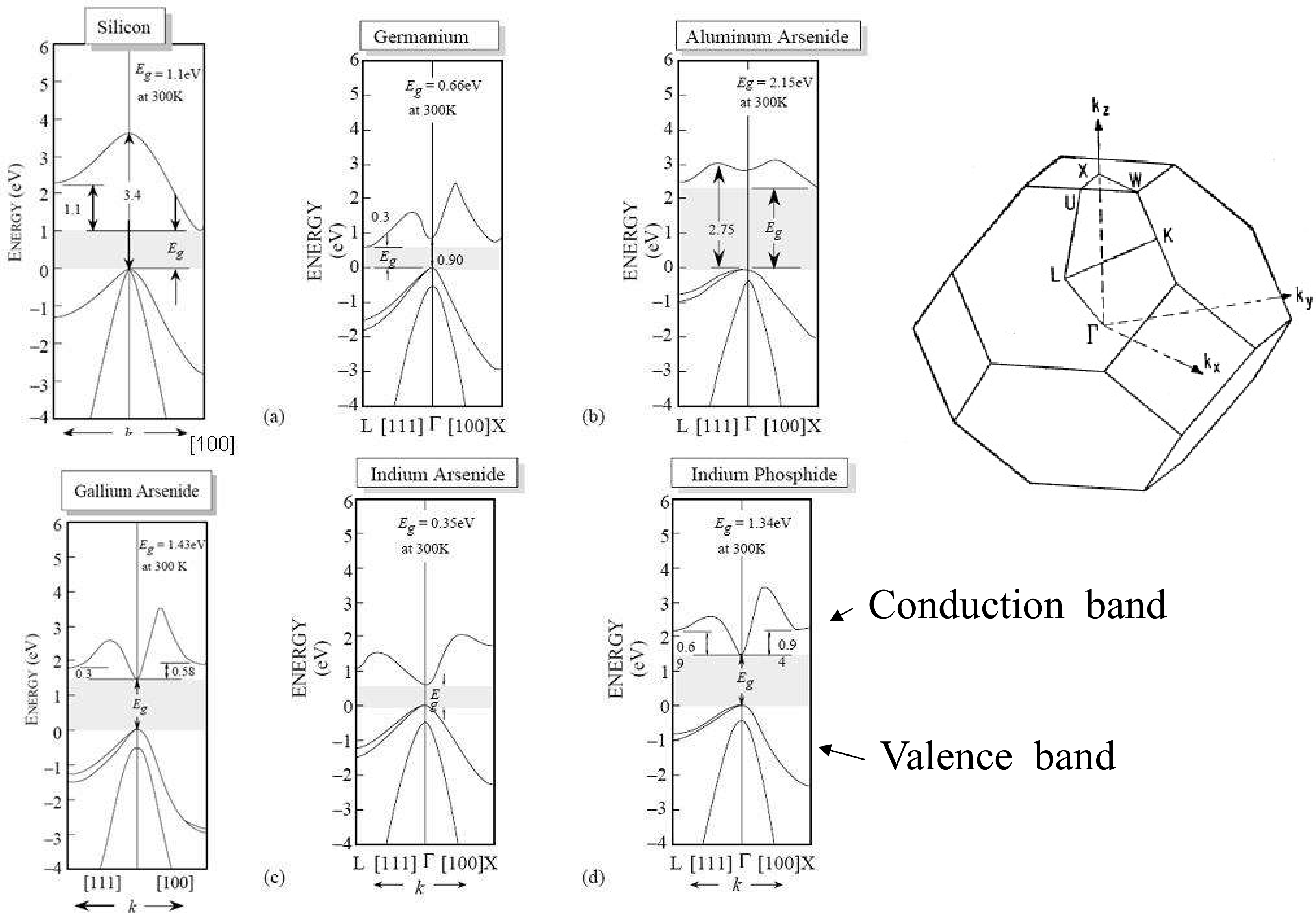


Direct bandgap

Indirect bandgap

Direct bandgap semiconductors are used for optoelectronics

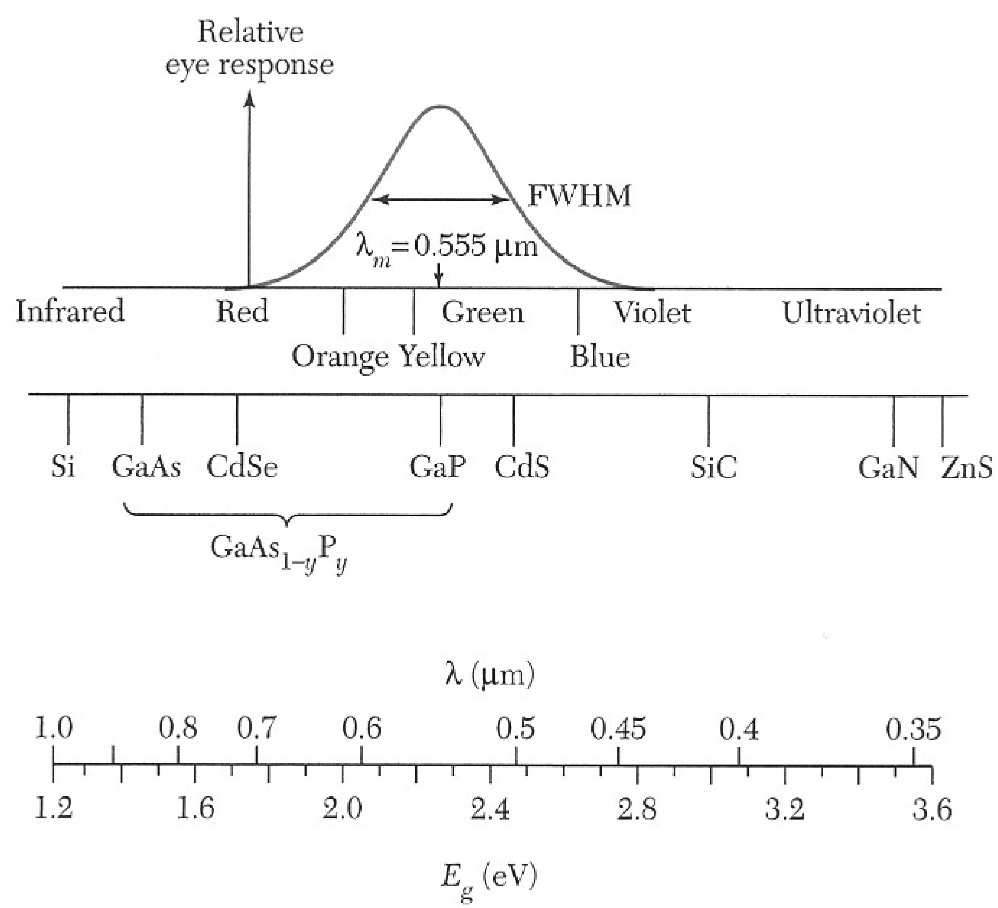
Semiconductors



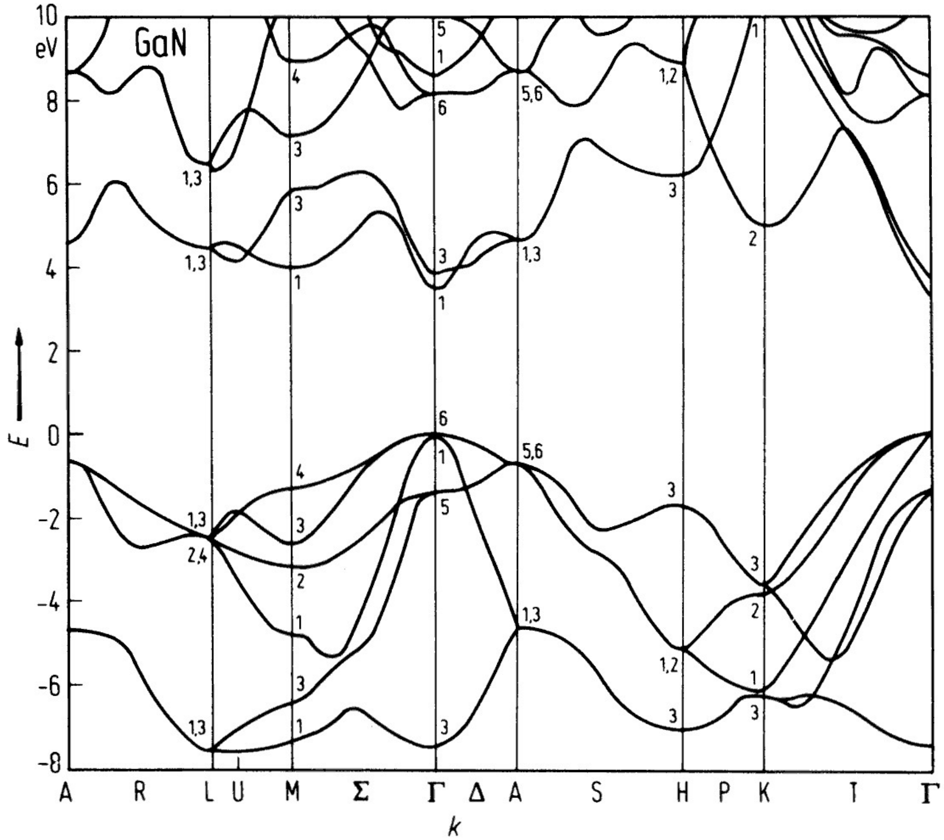
Light emitting diodes

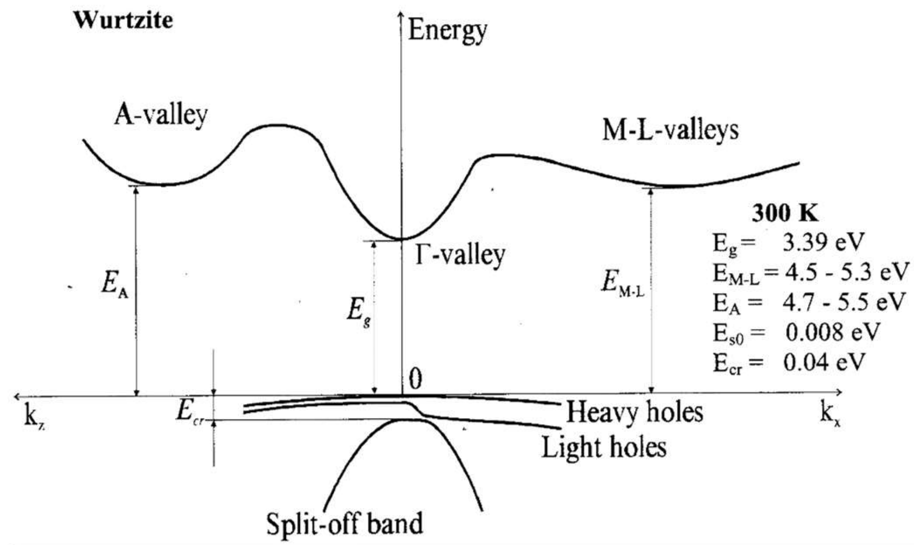
TABLE 1 Common III-V materials used to produce LEDs and their emission wavelengths.

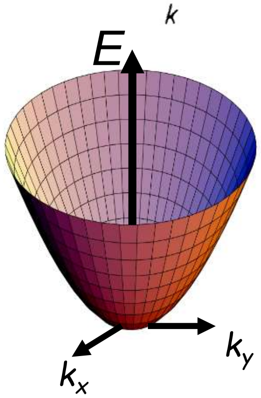
Material	Wavelength (nm)
InAsSbP/InAs	4200
InAs	3800
GaInAsP/GaSb	2000
GaSb	1800
$Ga_xIn_{1-x}As_{1-y}P_y$	1100-1600
$Ga_{0.47}In_{0.53}As$	1550
$Ga_{0.27}In_{0.73}As_{0.63}P_{0.37}$	1300
GaAs:Er,InP:Er	1540
Si:C	1300
GaAs:Yb,InP:Yb	1000
$Al_xGa_{1-x}As$:Si	650-940
GaAs:Si	940
$Al_{0.11}Ga_{0.89}As$:Si	830
$Al_{0.4}Ga_{0.6}As$:Si	650
$GaAs_{0.6}P_{0.4}$	660
$GaAs_{0.4}P_{0.6}$	620
$GaAs_{0.15}P_{0.85}$	590
$(Al_xGa_{1-x})_{0.5}In_{0.5}P$	655
GaP	690
GaP:N	550-570
$Ga_xIn_{1-x}N$	340,430,590
SiC	400-460
BN	260,310,490

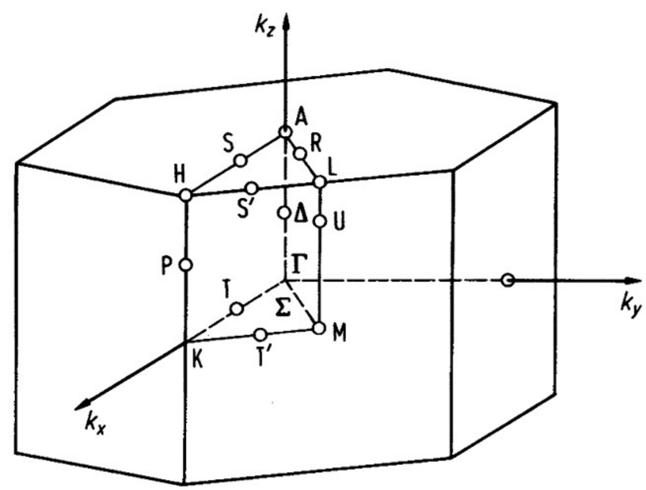


GaN





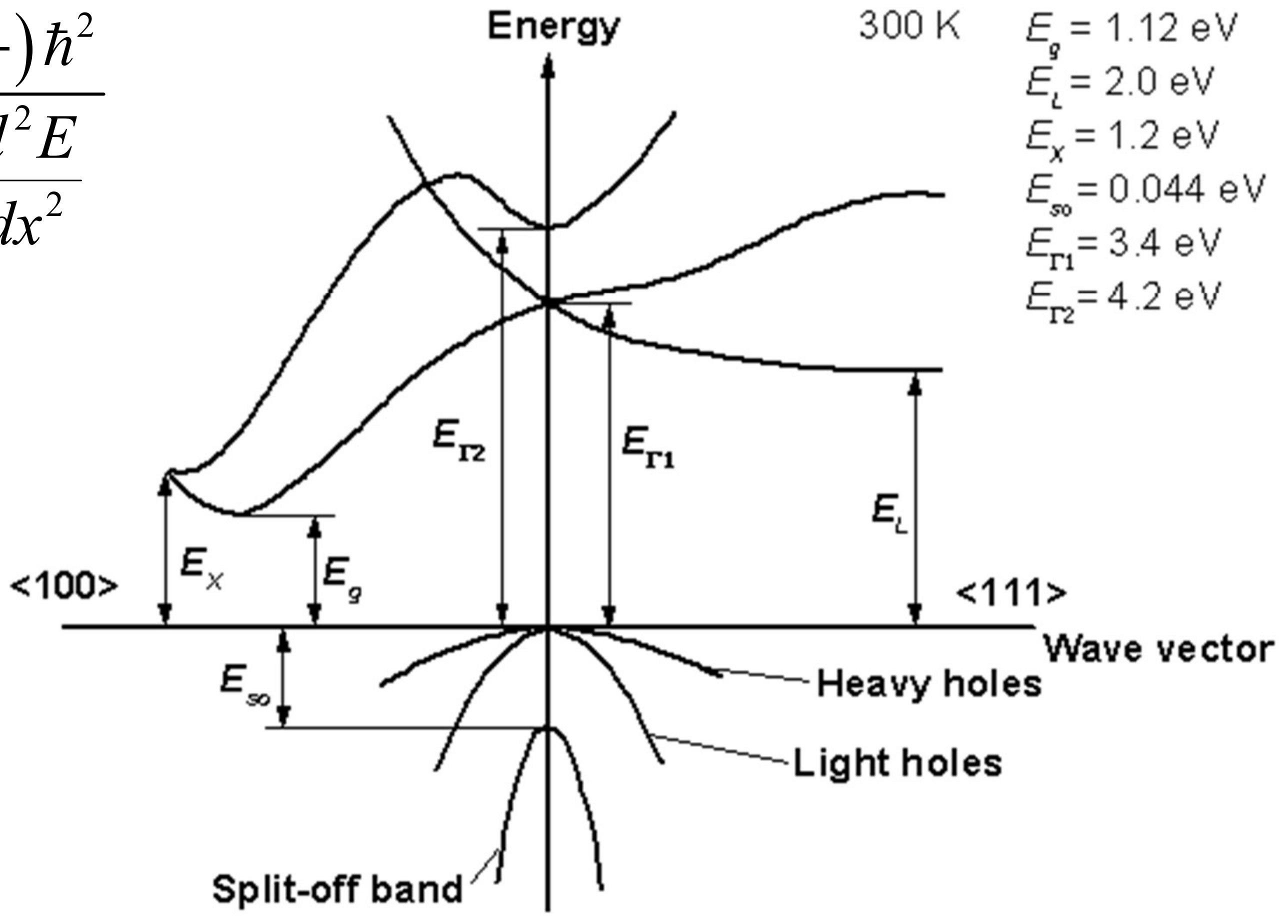




1st Brillioun zone of hcp

Silicon

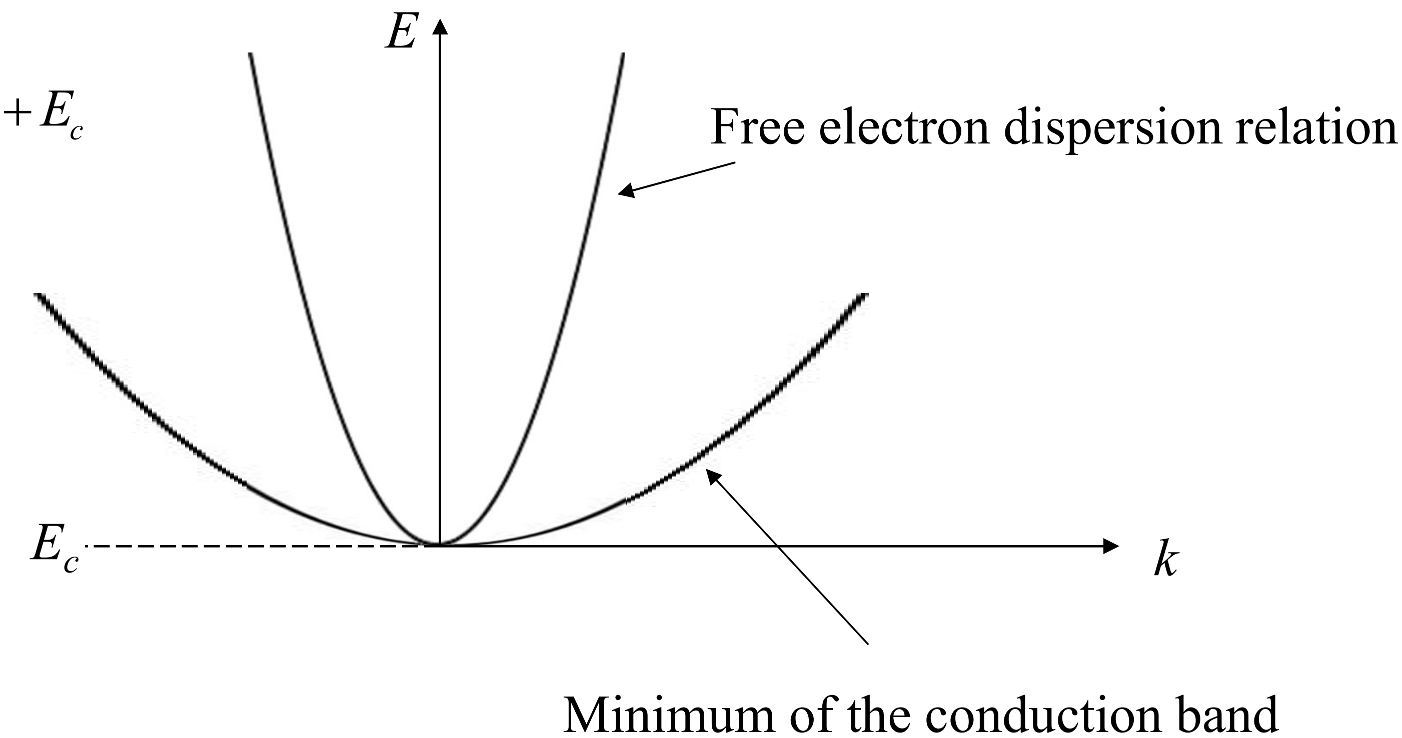
$$m^*_{e,h} = \frac{(-)\hbar^2}{\dfrac{d^2E}{dx^2}}$$



http://www.matprop.ru/Si_bandstr#Basic

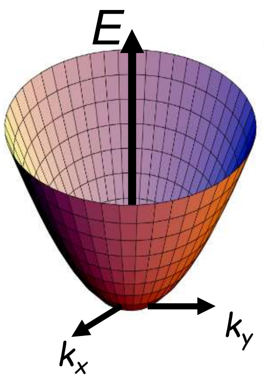
Conduction band minimum

$$E = \frac{\hbar^2 \left(\vec{k} - \vec{k}_0\right)^2}{2m^*} + E_c$$



Near the conduction band minimum, the bands are approximately parabolic.

Effective mass



$$E = \frac{\hbar^2 \left(\vec{k} - \vec{k}_0\right)^2}{2m^*} + E_c$$

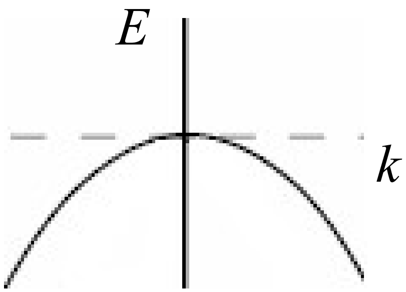
The parabola at the bottom of the conduction band does not have the same curvature as the free-electron dispersion relation. We define an effective mass to characterize the conduction band minimum.

$$m^* = \frac{\hbar^2}{\dfrac{d^2 E(\vec{k})}{dk_x^2}}$$

This effective mass is used to describe the response of electrons to external forces in the particle picture.

Top of the valence band

In the valence band, the effective mass is negative.



$$m^* = \frac{\hbar^2}{\frac{d^2E(\vec{k})}{dk_x^2}} < 0$$

Charge carriers in the valence band are positively charged holes.

m^*_h = effective mass of holes

$$m_h^* = \frac{-\hbar^2}{\frac{d^2E(\vec{k})}{dk_x^2}}$$

Holes

A completely filled band does not contribute to the current.

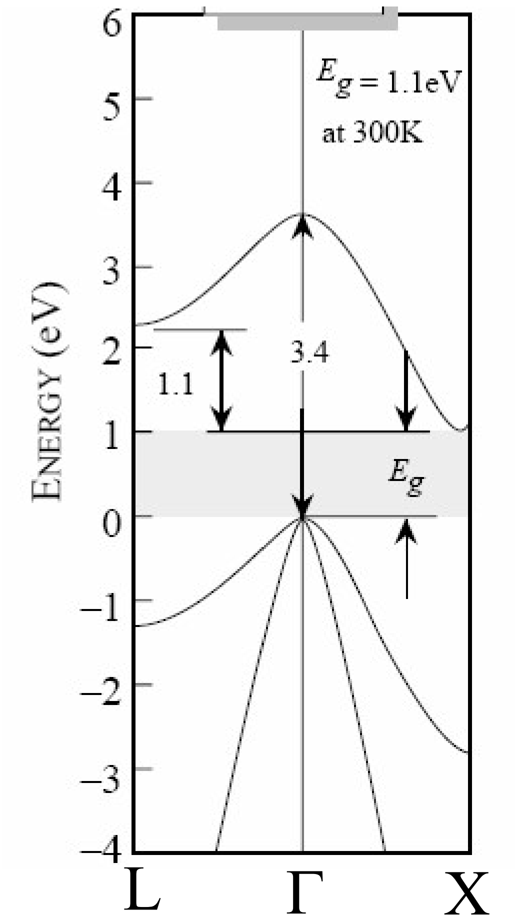
$$\vec{j} = \int_{\text{filled states}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k}$$

$$= \int_{\text{band}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k} - \int_{\text{empty states}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k}$$

$$= \int_{\text{empty states}} e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k}$$

Holes have a positive charge and a positive mass.

Effective Mass



$$E = \frac{\hbar^2 \left(\vec{k} - \vec{k}_0\right)^2}{2m^*} + E_c$$

$$m_e^* = \frac{\hbar^2}{\dfrac{d^2E}{dk_x^2}}$$

$$E = \frac{-\hbar^2 \left(\vec{k} - \vec{k}_0\right)^2}{2m^*} + E_v$$

$$m_h^* = \frac{-\hbar^2}{\dfrac{d^2E}{dk_x^2}}$$