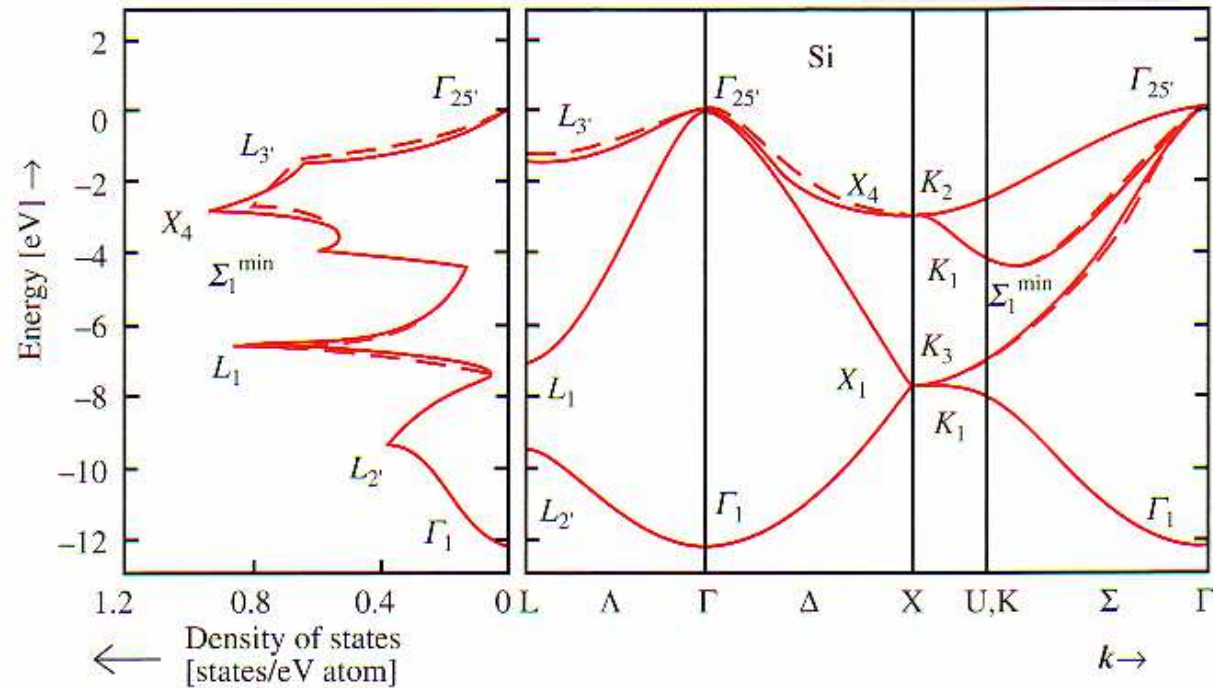
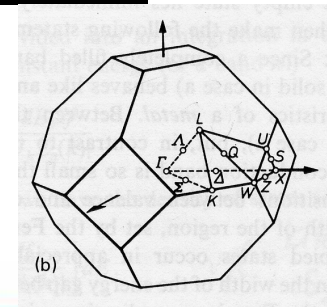


The Electronic Density of States

The concept:
 For non-crystalline solids (amorphous, organic,...) the electronic states are no Bloch waves. The crystal momentum k is no good quantum number any more. Electronic states can only be classified by their energy. This leads to the concept of **Density of Stats, DOS $D(E)$** .

$$D(E) = \frac{1}{L^d} \frac{dN}{dE}$$

in units of $\text{cm}^{-d} (\text{eV})^{-1}$



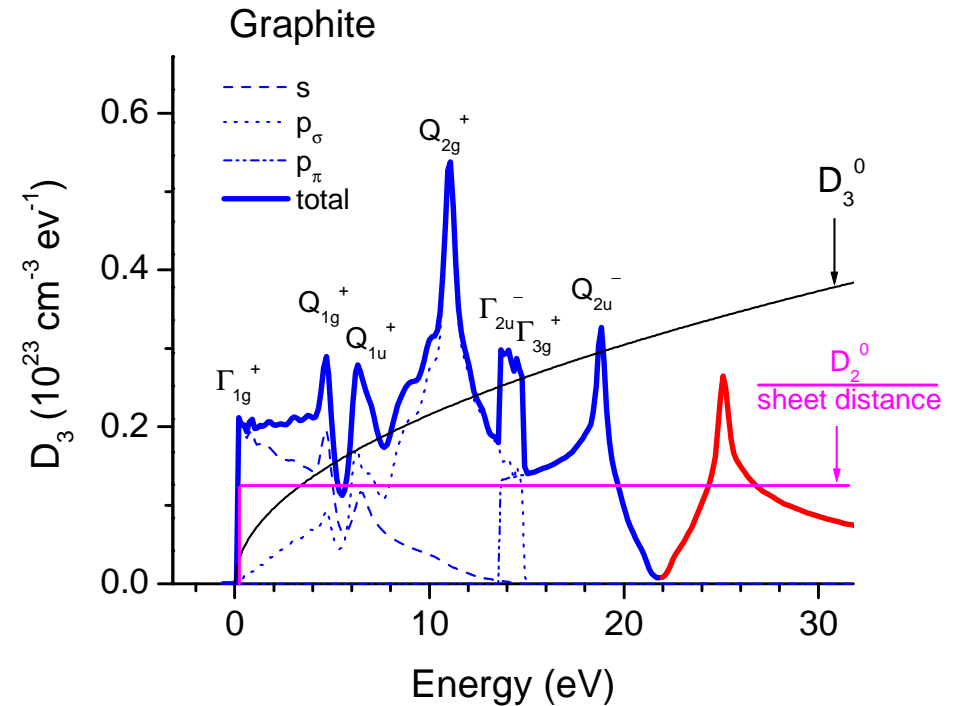
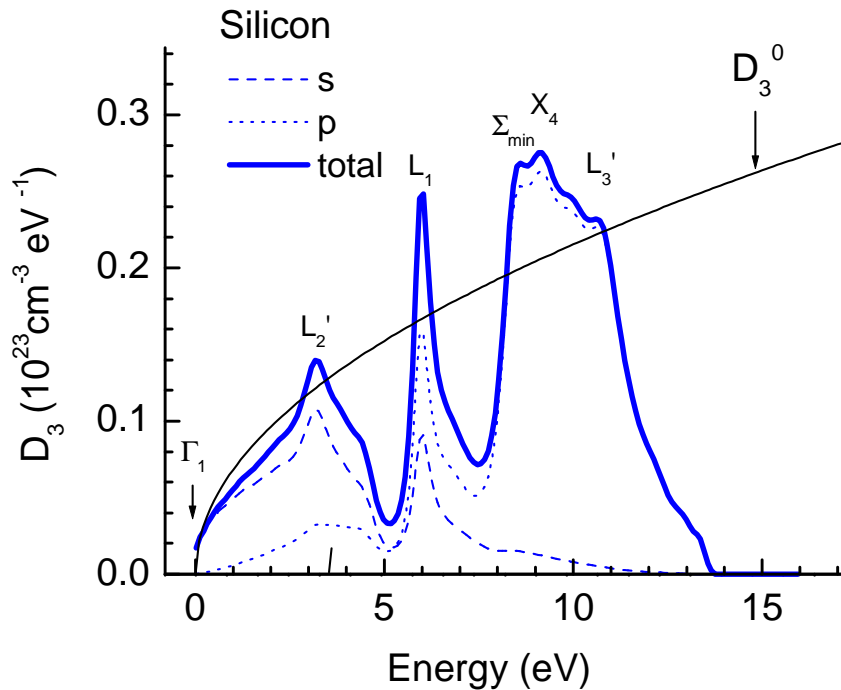
For crystalline solids, $D(E)$ can be extracted from the band structure function:

$$D(E) = \frac{2}{(2\pi)^3} \sum_n \int_{\text{constant energy surface}} \frac{dA_k}{|\nabla_{\vec{k}} E_n(\vec{k})|}$$

for $d=3$ and analogous for $d=2,1$

Note: $D(E)$ large when the bands are flat! \rightarrow „van-Hove singularities“ when $\nabla_{\vec{k}} E_n(\vec{k}) = \vec{0}$

Examples



Note:

- Peaks (= van Hove singularities) are labelled with **symmetry notations for the corresponding wave functions.**
- DOS is represented as the sum of **partial densities of states** of different orbital character!

The Effective Mass Approximation

1. Valence bands in Zincblende and Diamond type S.C.: light hole, heavy hole and spin-orbit splitt-off band.

	A	B	C ²	Δ ₀ [eV]	m _{hh} /m ₀		m _{lh} /m ₀		m _{so} /m ₀	
					exp	th	exp	th	exp	th
C ^b	-2.5	0.2	4.6	0.013 ^a		0.66 ^c		0.29 ^c		0.39 ^b
Si ^c	-4.28	-0.68	24	0.044	0.54	0.50	0.15	0.15	0.23	0.24
Ge	-13.38	-8.5	173	0.295	0.34	0.43	0.043	0.041	0.095	0.1
SiC ^c	-2.8	-1.016	5.8	0.014		0.6		0.25		0.36
GaN ^d	-5.05	-1.2	34	0.017		0.5 ^e		0.13 ^e		0.2
GaP ^c	-4.05	-0.98	16	0.08	0.57	0.51	0.18	0.16		0.25
GaAs	-6.9	-4.4	43	0.341	0.53	0.73	0.08	0.08	0.15	0.17
GaSb	-13.3	-8.8	230	0.75	0.8	0.98	0.05	0.04		0.15
InP ^c	-5.15	-1.9	21	0.11	0.58	0.44	0.12	0.11	0.12	0.2
InAs	-20.4	-16.6	167	0.38	0.4	0.4	0.026	0.026	0.14	0.10
InSb	-36.41	-32.5	43	0.81	0.42	0.48	0.016	0.013		0.12
ZnS	-2.54	-1.5		0.07						
ZnSe	-2.75	-1.0	7.5	0.43		1.09		0.145		
ZnTe	-3.8	-1.44	14.0	0.93						
CdTe	-4.14	-2.18	30.3	0.92						

m = m₀ =
free electron
mass

Source:
Yu/Cardona

$$E_{hh/lh}(\vec{k}) = \frac{\hbar^2}{2m} \left\{ Ak^2 + /- \sqrt{B^2k^4 + C^2(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2)} \right\} \quad \text{and} \quad E_{so}(\vec{k}) = -\Delta_0 - \frac{\hbar^2}{2m_{so}} k^2$$

For the direction-averaged effective masses:

$$\frac{m}{m_{hh}} = -A + B \cdot f\left(\frac{C^2}{B^2}\right) \quad \text{and} \quad \frac{m}{m_{lh}} = -A - B \cdot f\left(\frac{C^2}{B^2}\right) \quad \text{with different function } f^*$$

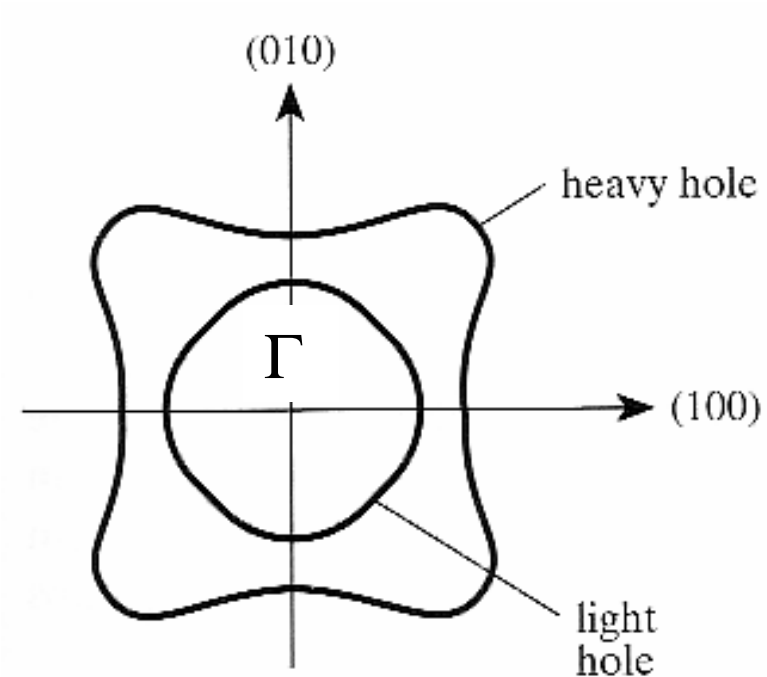
See Yu/Cardona, pages 81, 200, 201

The Effective Mass Approximation

$$E_{\text{hh/lh}}(\vec{k}) = \frac{\hbar^2}{2m} \left\{ Ak^2 + /- \sqrt{B^2 k^4 + C^2 (k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2)} \right\}$$

Constant energy surfaces of the $j=3/2$ -like valence bands

Section of constant energy surfaces with the k_x - k_y -plane in k -space



The Effective Mass Approximation

Conduction bands in Zincblende and Diamond type S.C.: the direct and indirect band gap case

1. the direct band gap case:

Isotropic, quadratic bands mostly with small effective masses m_c

Examples:

GaAs	$m_c = 0,070 m$
GaSb	0,047
InSb	0,015
InAs	0,026
InP	0,073

2. the indirect band gap case:

CBM at \vec{k}_0 on symmetry line in BZ. Uniaxial effective mass tensor with longitudinal and transverse effective masses:

Valley degeneracy corresponding to the star of \vec{k}_0

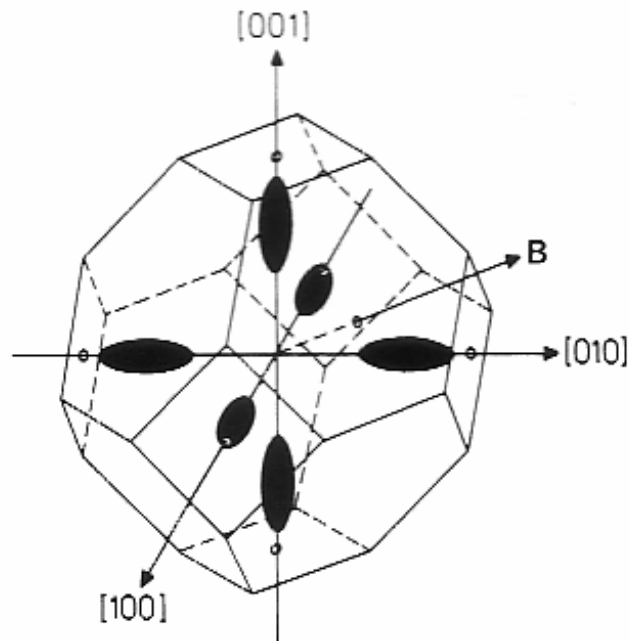
$$E(\vec{k}) = E(\vec{k}_0) + \frac{\hbar^2}{2m_t} \left| (\vec{k} - \vec{k}_0)_\perp \right|^2 + \frac{\hbar^2}{2m_\ell} \left| (\vec{k} - \vec{k}_0)_\parallel \right|^2$$

Examples:

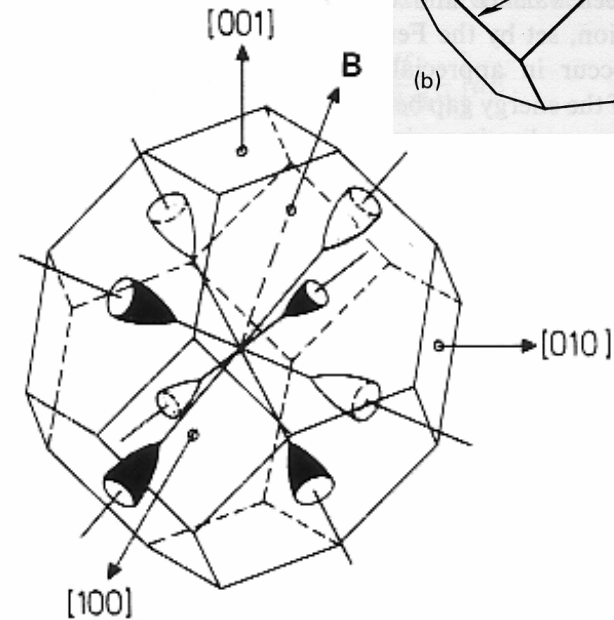
Si	$m_\parallel = 0,19 m$,	$m_\perp = 0,92 m$
Ge	$m_t = 0,082 m$,	$m_\ell = 1,57 m$

The Effective Mass Approximation

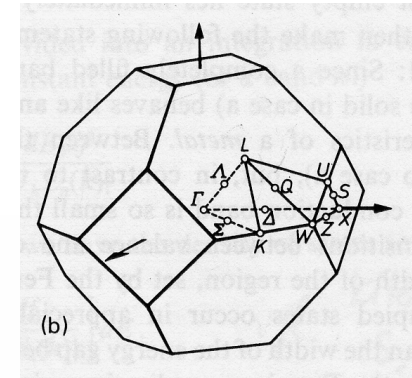
Conduction band constant energy surfaces for Si and Ge



Si: \vec{k}_0 on Δ inside BZ



Ge: \vec{k}_0 at L on BZ boundary



$$E(\vec{k}) = E(\vec{k}_0) + \frac{\hbar^2}{2m_t} \left| (\vec{k} - \vec{k}_0)_\perp \right|^2 + \frac{\hbar^2}{2m_l} \left| (\vec{k} - \vec{k}_0)_\parallel \right|^2$$