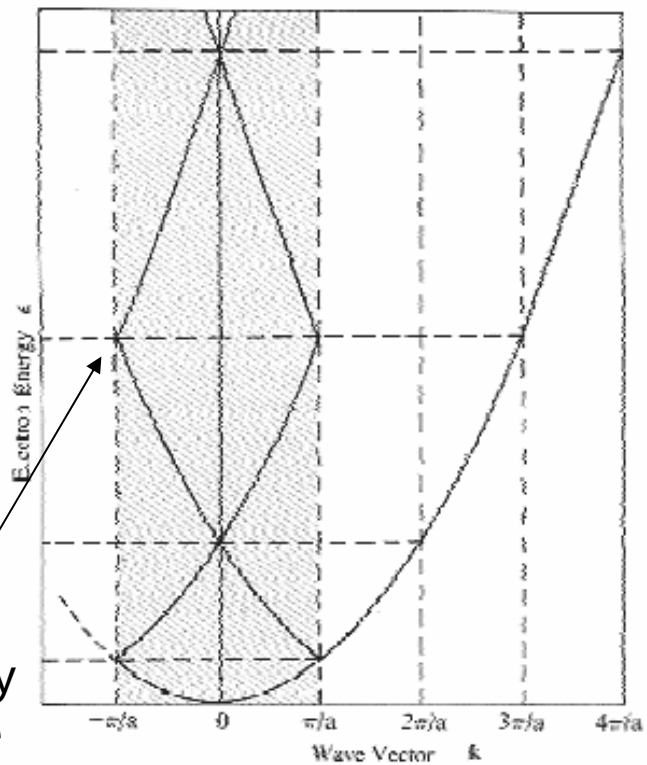
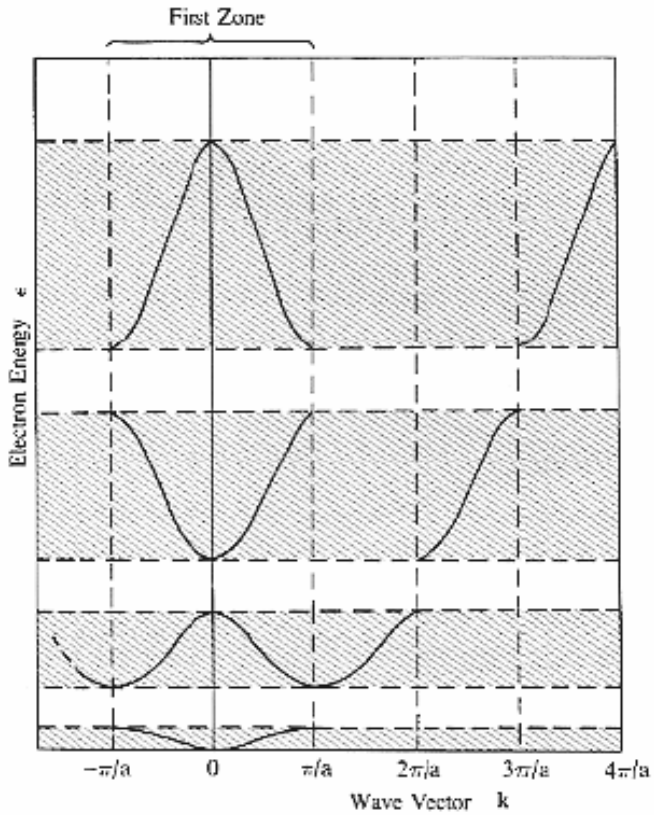
Nearly free electron model

Using free electron wave functions as the basis



Free particle

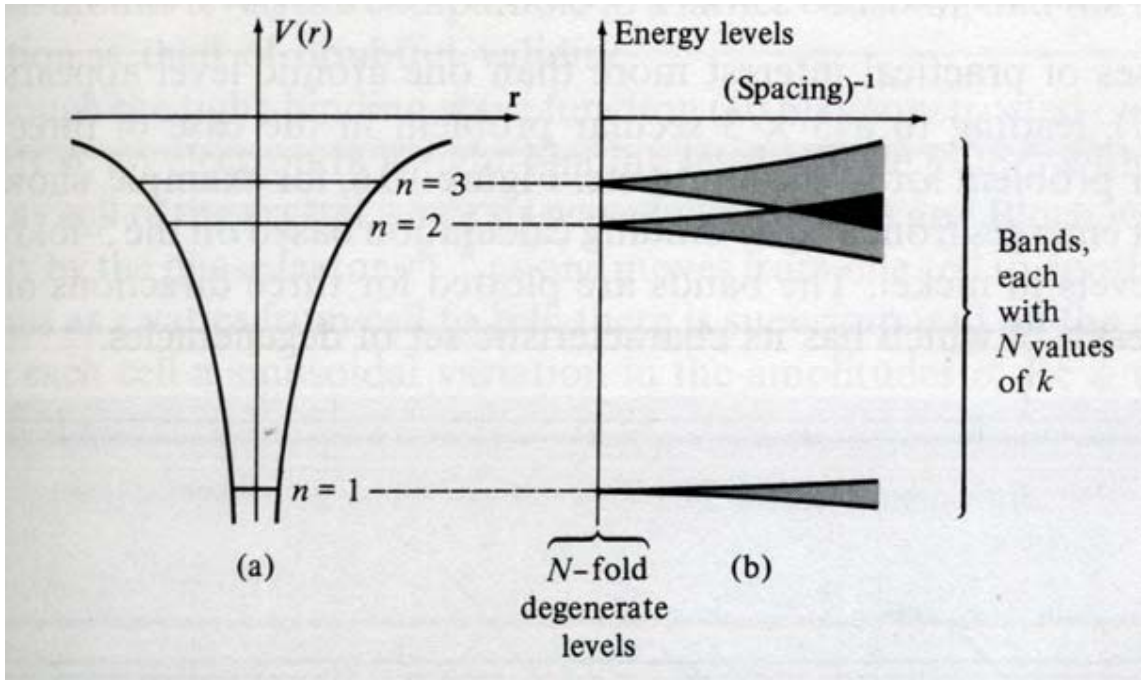


Weak periodic potential

degeneracy at the zone boundaries

Tight binding method (LCAO, Linear Combinations of Atomic Orbitals)

Using the atomic orbitals as the basis



N-fold degeneracy lifted due to the overlap of wave functions between neighboring atoms

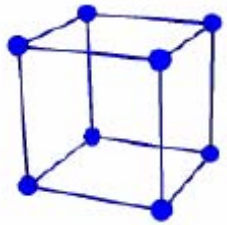
Widely used in actual calculation of band structures in solids

Common crystal structures

http://cst-www.nrl.navy.mil/lattice/
http://www.chem.ox.ac.uk/icl/heyes/structure_of_solids/Strucsol.html
http://home3.netcarrier.com/~chan/SOLIDSTATE/CRYSTAL/

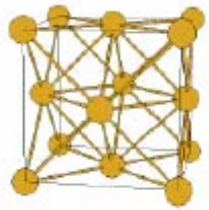
Simple cubic

$a(1,0,0)$
$a(0,1,0)$
$a(0,0,1)$



Face-centered cubic

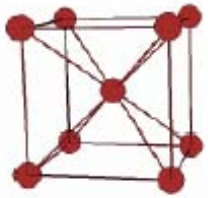
$a/2(0,1,1)$
$a/2(1,0,1)$
$a/2(1,1,0)$



Al, Cu, Ni, Sr, Rh, Pd, Ag,
Ce, Tb, Ir, Pt, Au, Pb, Th

Body-centered cubic

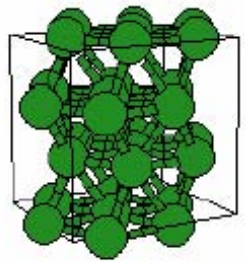
$a/2(-1,1,1)$
$a/2(1,-1,1)$
$a/2(1,1,-1)$



W, Li, Na, K, V, Cr, Fe, Rb,
Nb, Mo, Cs, Ba, Eu, Ta

Hexagonal close-packed

$a/2(1,-3^{1/2},0)$
$a/2(1, 3^{1/2},0)$
$c(0,0,1)$

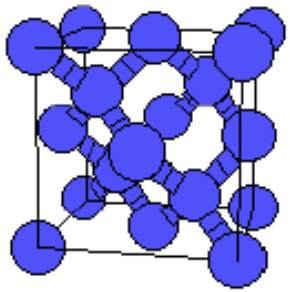


Mg, Be, Sc, Te, Co, Zn, Y,
Zr, Tc, Ru, Gd, Tb, Py, Ho,
Er, Tm, Lu, Hf, Re, Os, Tl

Common crystal structures II - semiconductors

Diamond

$a/2(0,1,1)$
$a/2(1,0,1)$
$a/2(1,1,0)$



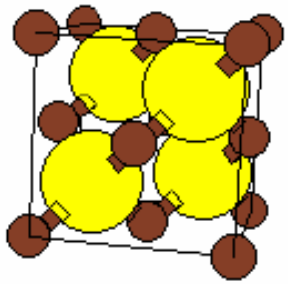
Two interpenetrating fcc lattices displaced by 1/4 a.

Result of all sp^3 covalent bonds.

C, **Si**, **Ge**, Sn

Zinc blende

$a/2(0,1,1)$
$a/2(1,0,1)$
$a/2(1,1,0)$



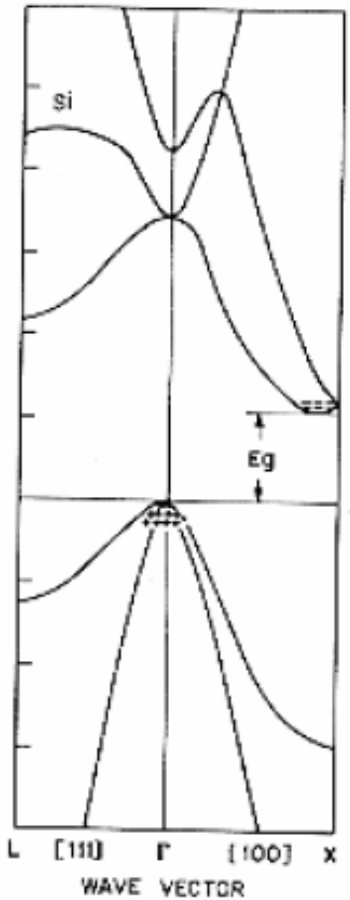
Two interpenetrating fcc lattices displaced by 1/4 a, each lattice a different species.

ZnS, AgI, **AlAs**, **AlP**, **AlSb**, BAs, BN, BP, BeS, BeSe, BeTe, **CdS**, CuBr, CuCl, CuF, CuI, **GaAs**, **GaP**, **GaSb**, HgS, HgSe, HgTe, **InAs**, **InP**, MnS, MnSe, **SiC**, **ZnSe**, ZnTe

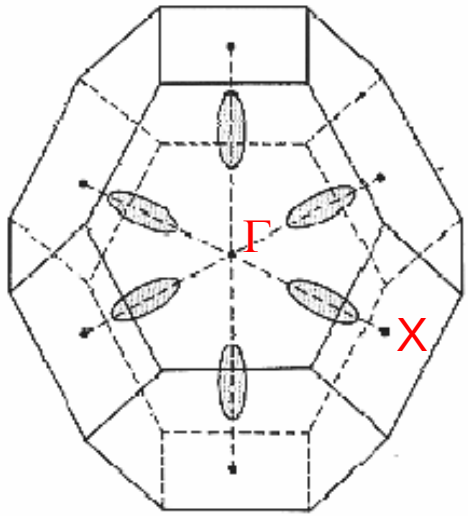
Common materials - silicon

s-like conduction band, p-like valence band

Heavy and light hole bands



From Sze



constant energy surfaces

From Blakemore

$E_g = 1.12$ eV at 300 K

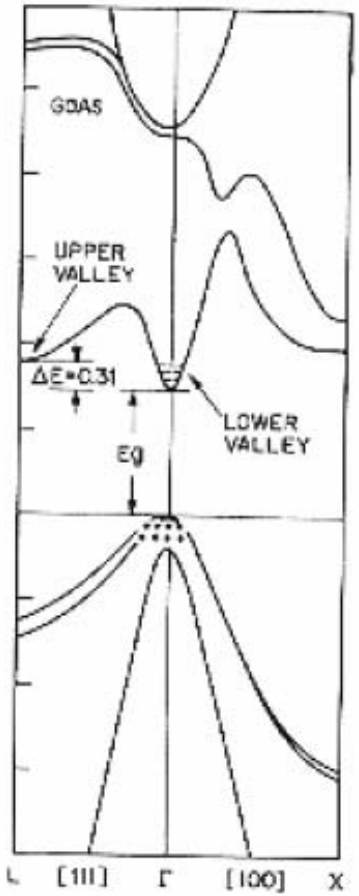
Electron $m_* = 0.98\ m_0$ long., $0.19\ m_0$ trans.

Hole $m_* = 0.16\ m_0$ light, $0.49\ m_0$ heavy.

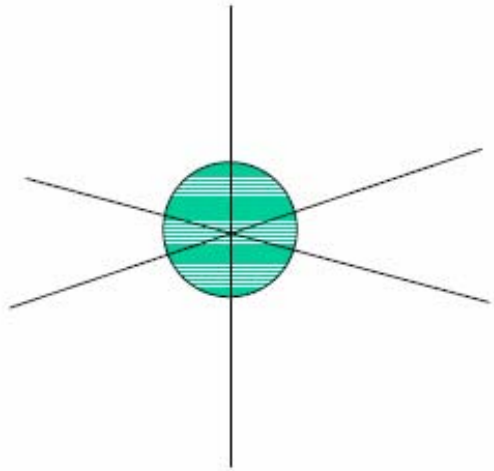
6-fold “Valley degeneracy due to the 6 X-points

Γ, center of the Brillouin zone. L,X center of the hexagons and squares, respectively

Common materials: GaAs



From Sze



E_g = 1.42 eV at 300 K

Electron $m_* = 0.067\ m_0$

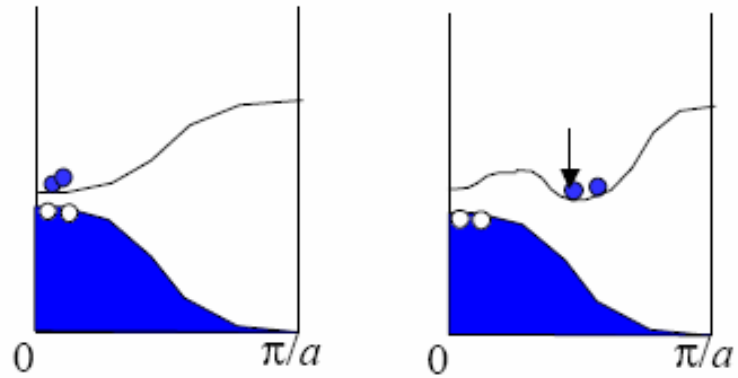
Hole $m_* = 0.082\ m_0$

Electrons in GaAs conduction band form spherical Fermi surface - easy to think about.

Electrons and Holes III

Semiconductors

- Require an energy at least as large as E_g to create an electron-hole pair.
- Electrons and holes are in different bands.



- Optical processes often used to create e-h pairs, with photon energy $\hbar\omega > \sim E_g$.
- Indirect gap case: need an additional excitation to conserve momentum.
- Result: GaAs, InP (direct gap) semiconductors used in photodetectors + LEDs; Si & Ge are not.
- Nanostructuring can allow some rules to be bent - light emission from nanoporous Si.