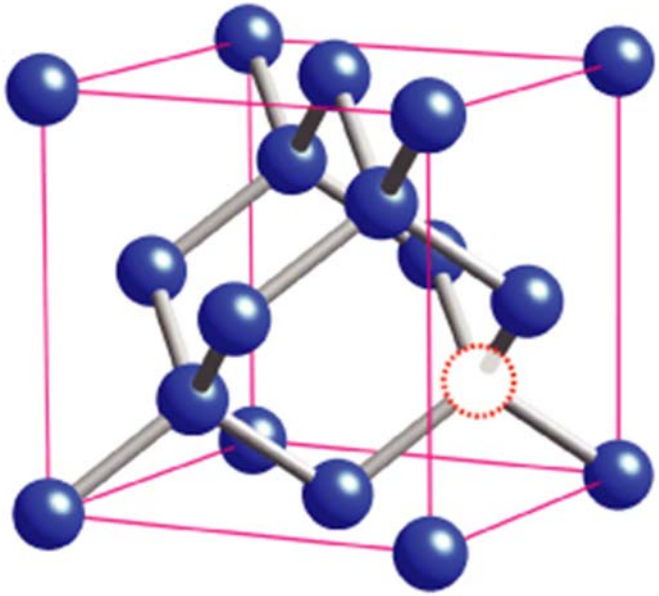
Condensed Matter Physics: Important Concepts

- crystal structure of Si, Ge, GaAs, III-V's
- semiconductor bandstructure
- effective mass approximation
- valence bands and spin-orbit coupling
- density of state
- doping

Condensed Matter Physics: Important Concepts

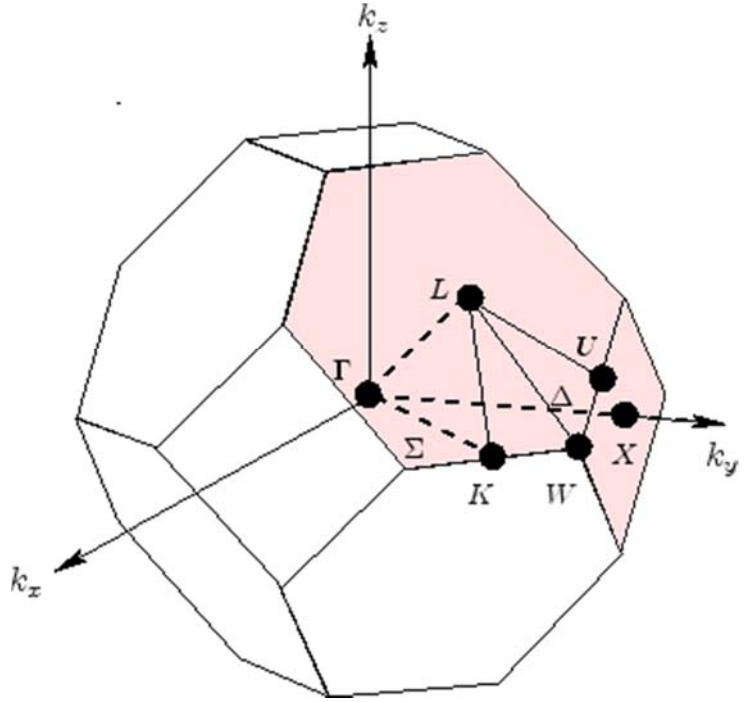
Silicone (Si)



diamond structure of Si

face centered cubic lattice
two atomic base:
(0,0,0) and (a/4, a/4, a/4)

a = 5.65 Å

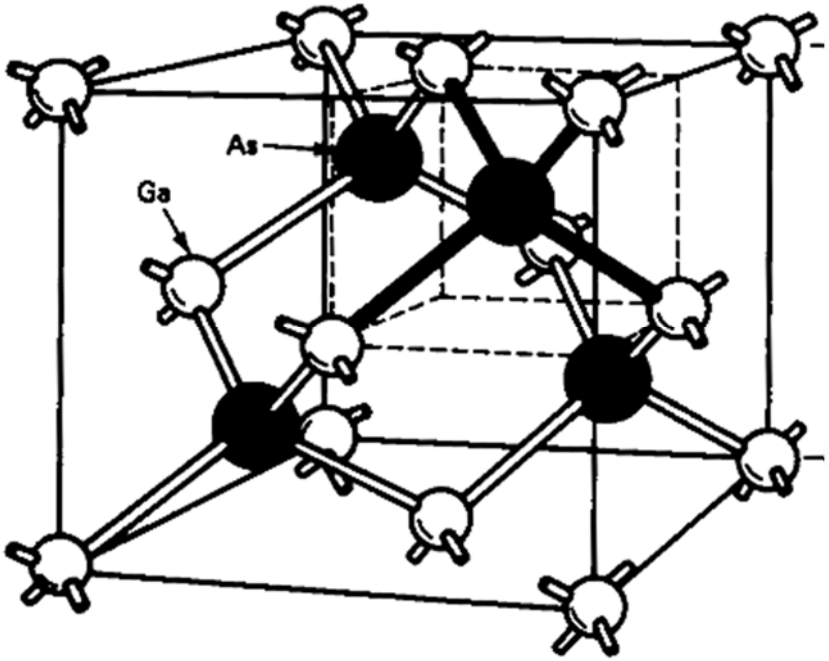


brillouin zone
(bcc)

column IV material

Ge also has diamond structure

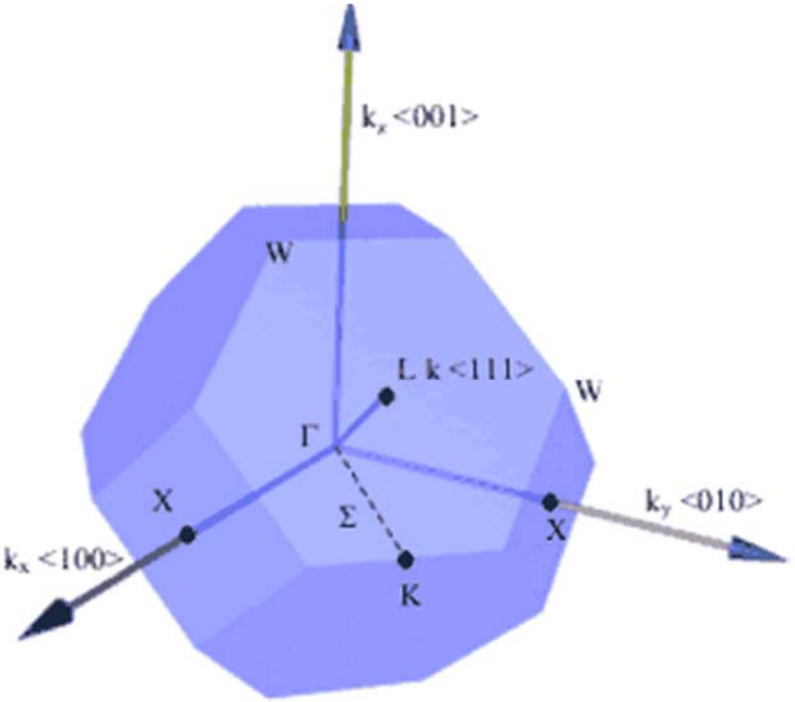
Gallium Arsenide (GaAs)



zincblende structure of GaAs

dito Si,
but one atom Ga, one As

a = 5.43 Å



brillouin zone
(bcc)

III – V semiconductor
(binary compound)

II	III	IV	V	VI
	5 2 3 **B** Boron 10.811	6 2 4 **C** Carbon 12.0107	7 2 5 **N** Nitrogen 14.0067	8 2 6 **O** Oxygen 15.9994
	13 2 8 3 **Al** Aluminium 26.9815386	14 2 8 4 **Si** Silicon 28.0855	15 2 8 5 **P** Phosphorus 30.973762	16 2 8 6 **S** Sulfur 32.065
30 2 8 18 2 **Zn** Zinc 65.38	31 2 8 18 3 **Ga** Gallium 69.723	32 2 8 18 4 **Ge** Germanium 72.63	33 2 8 18 5 **As** Arsenic 74.9216	34 2 8 18 6 **Se** Selenium 78.96
48 2 8 18 18 2 **Cd** Cadmium 112.411	49 2 8 18 18 3 **In** Indium 114.818	50 2 8 18 18 4 **Sn** Tin 118.71	51 2 8 18 18 5 **Sb** Antimony 121.76	52 2 8 18 18 6 **Te** Tellurium 127.6
80 2 8 18 32 18 2 **Hg** Mercury 200.59	81 2 8 18 32 18 3 **Tl** Thallium 204.3833	82 2 8 18 32 18 4 **Pb** Lead 207.2	83 2 8 18 32 18 5 **Bi** Bismuth 208.9804	84 2 8 18 32 18 6 **Po** Polonium (209)

III-V binaries
zinc-blende

II-VI binaries, also zinc-blende

Bands

Electrons obey the Schrödinger equation (neglecting interactions)

$$\left\{-\frac{\hbar^2}{2m}\Delta + V(\vec{r})\right\} \psi(r) = \varepsilon\, \psi(r) \qquad (1)$$

$\psi(\vec{r})$: wave function

$V(\vec{r})$: periodic potential $U(\vec{r}+\vec{R}) = U(\vec{r})$

free electrons: $V \equiv 0 \rightarrow E = \frac{\hbar^2 k^2}{2m}$ $\psi = e^{i\vec{k}\vec{r}}$ plane wave

↳ parabolic dispersion

in periodic potential;

periodically, Bloch theorem:

2

$$\psi(r) = \psi_k(\vec{r}) = e^{ik\cdot r}\, u_k(r) \qquad (2)$$

with $u_k(r+R) = u_k(r)$ (3)

put (2) in (1), get

$$\left\{\frac{\hbar^2}{2m}(-i\nabla + k)^2 + U(r)\right\} u_k(r) = \varepsilon_k\, u_k(r) \qquad (4)$$

with periodic boundary conditions. (3)

Eigenvalue problem. finite size: discrete spectrum, energy bands: $\varepsilon_n(k)$
k: limited to first Brillouin zone
$\varepsilon_k = \varepsilon_{n,k}$ $\psi = \psi_{nk}(r)$

metals, semiconductors, insulators…

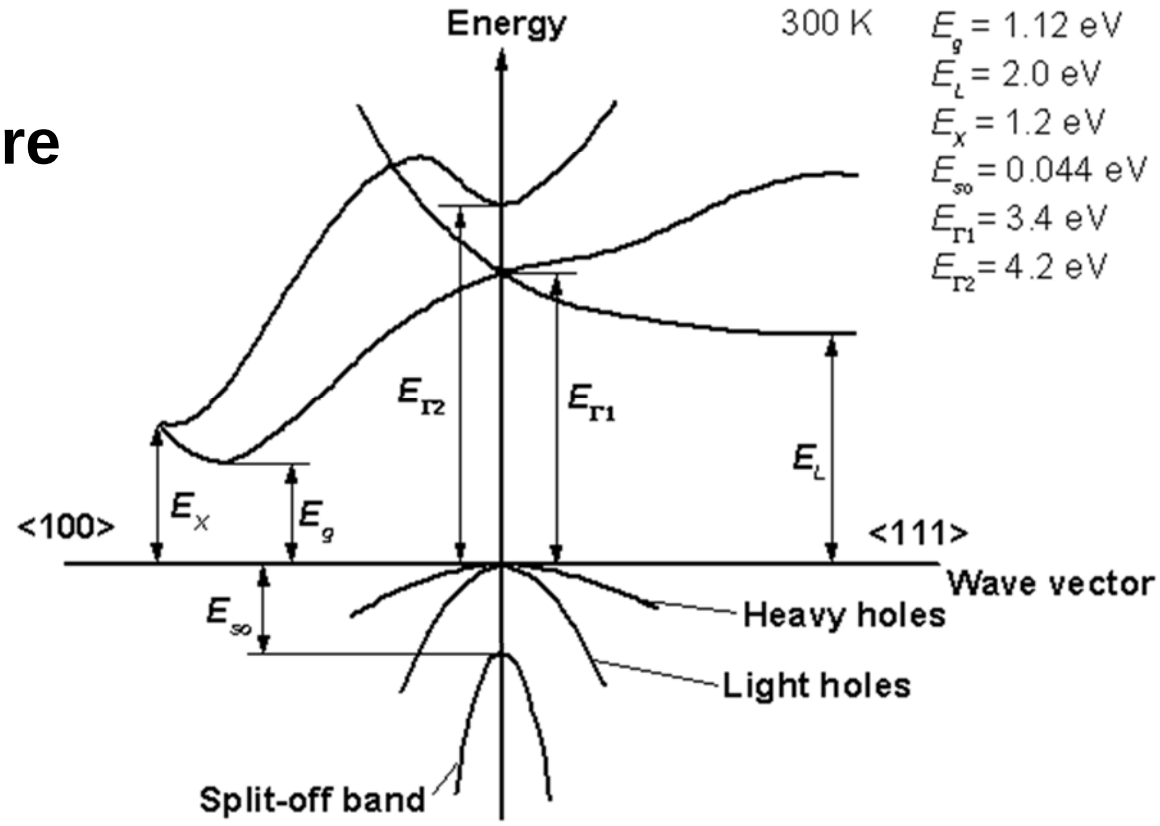
metals, semiconductors, insulators…

exact solution usually impossible, but approximations exist.

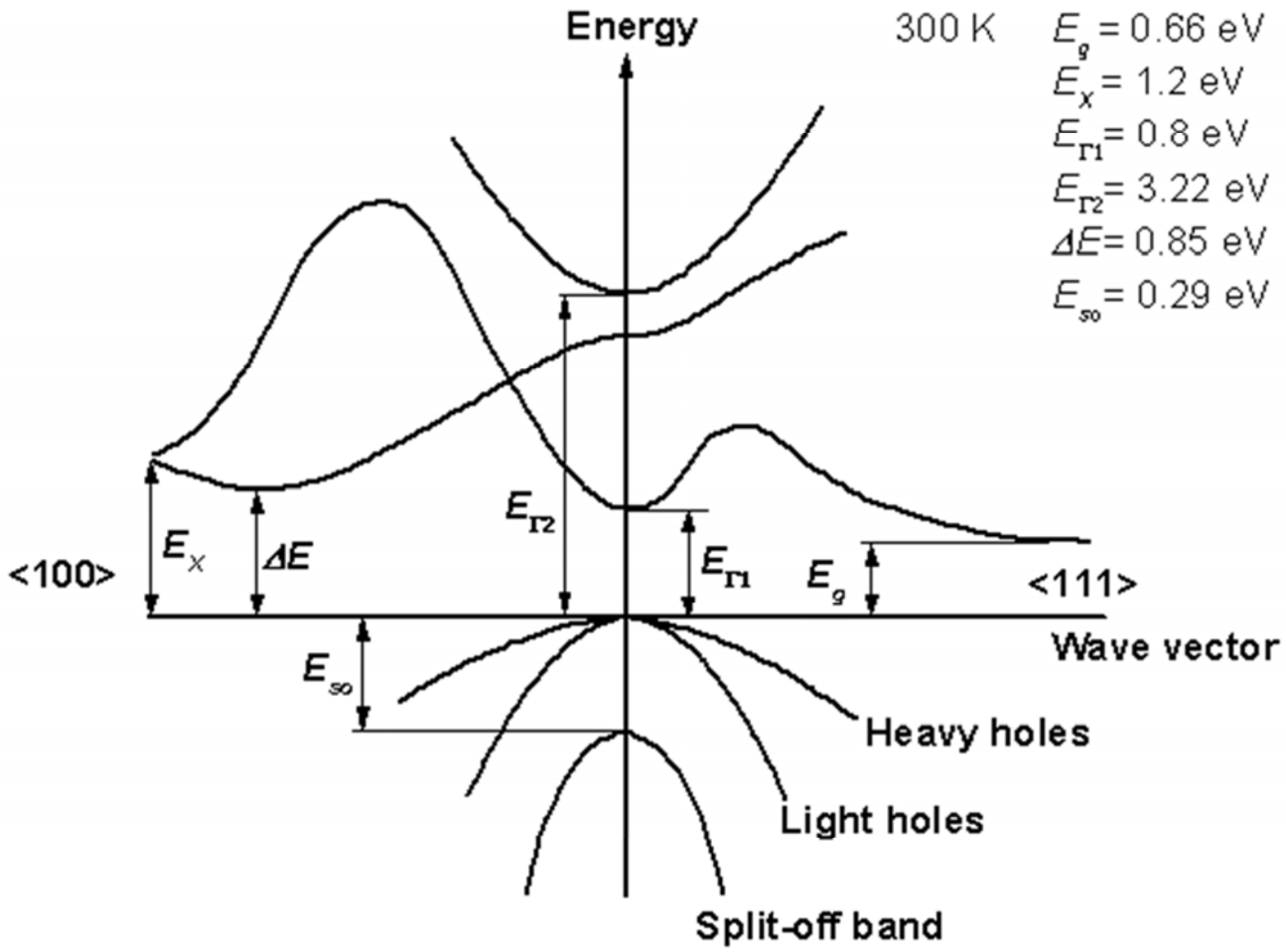
Si (covalent): indirect gap
GaAs (polar): direct gap

momentum missmatch for photons
optically active

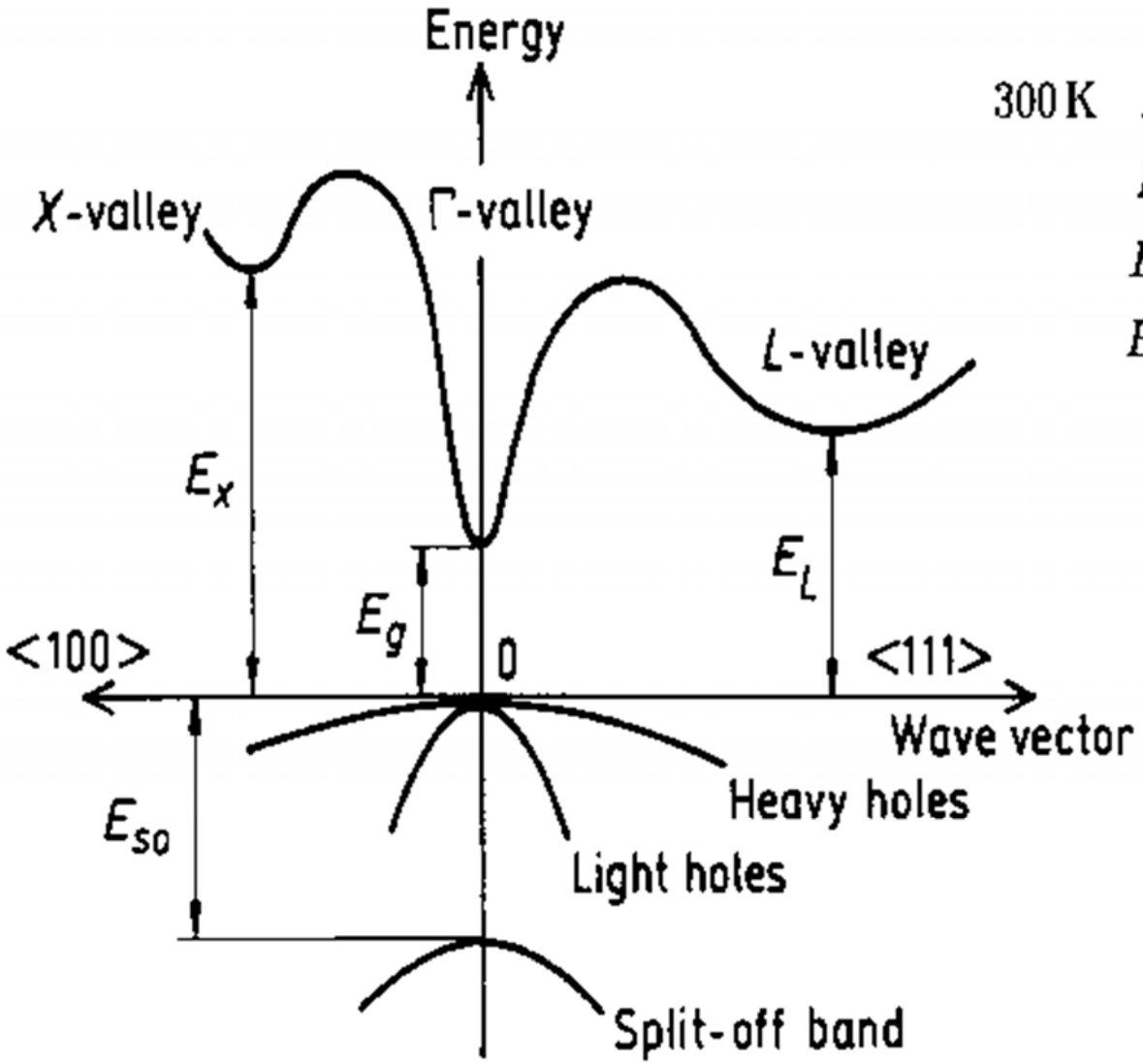
Si band structure



Ge band structure



GaAs band structure



300 K $E_g = 1.42$ eV

$E_L = 1.71$ eV

$E_X = 1.90$ eV

$E_{so} = 0.34$ eV

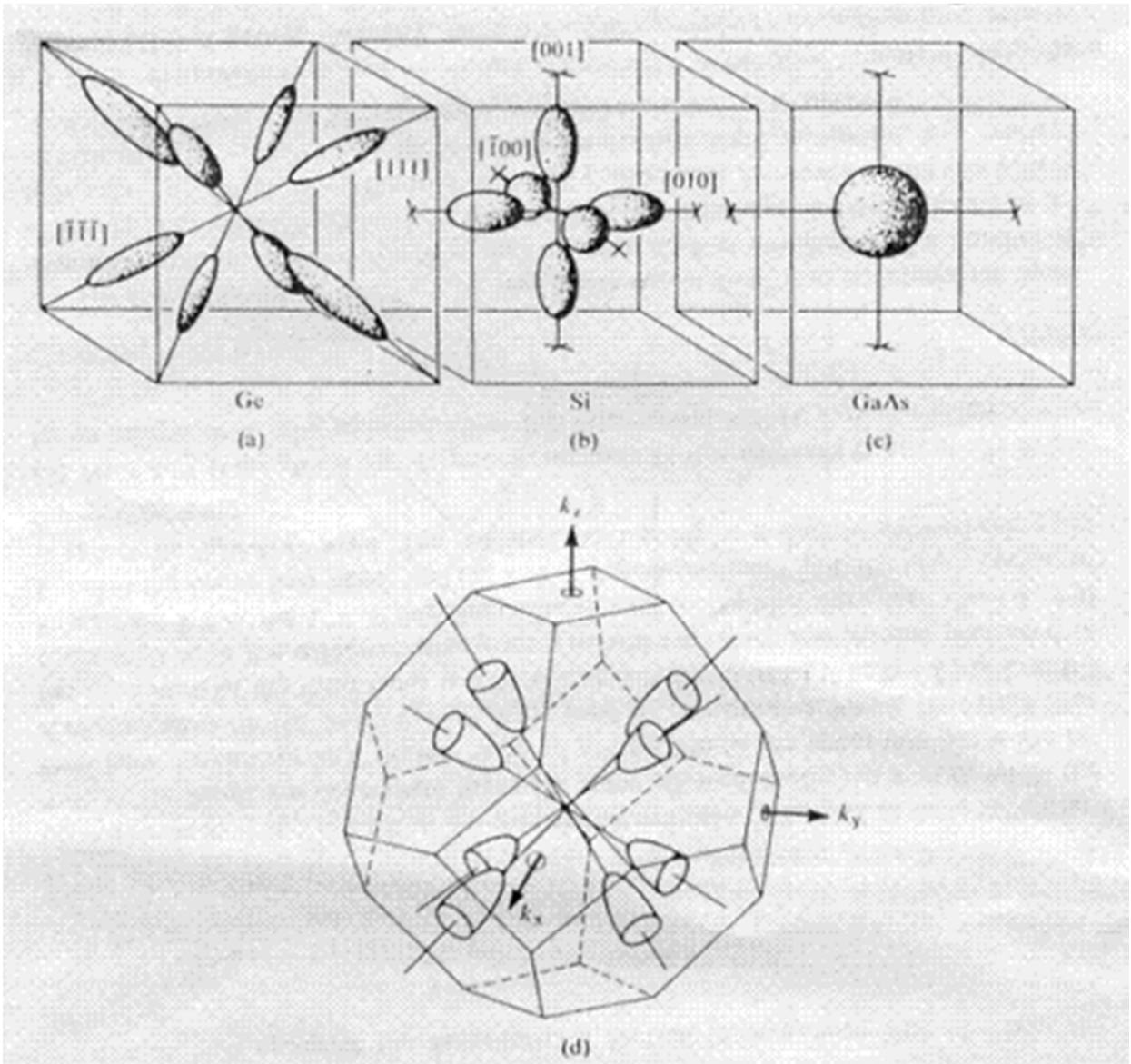


Fig. 3.14 Constant-energy surfaces characterizing the conduction-band structure in (a, d) Ge, (b) Si, and (c) GaAs. (d) shows the truncation of the Ge surfaces at the Brillouin-zone boundaries. [(a-c) after Sze[12] and Ziman;[13] (d) from McKelvey.[14] Reprinted with permission; the latter from Robert E. Krieger Publishing Co., Malabar, Florida.]

Effective mass approximation

Valence bands

built from atomic p states

3 fold orbital degeneracy plus spin: degeneracy 6

spin-orbit coupling: relativistic effect (Dirac equation)
motion of electron in electric field: Lorentz transformation gives magnetic field component: couples to spin via Zeeman term

$$H_{SO} = \frac{\hbar}{4m^2c^2}\vec{\sigma} \cdot \vec{\nabla} V \times \vec{p}$$

in spherically symmetric potential

$$H_{SO} \sim \vec{L} \cdot \vec{S}$$

assume electrons in solid behave as individual atoms:
p-states: L=1, S=1/2

Valence bands (2)

p-states: L=1, S=1/2
addition of angular momenta

$$1 \otimes \frac{1}{2} = \frac{3}{2} \oplus \frac{1}{2}$$

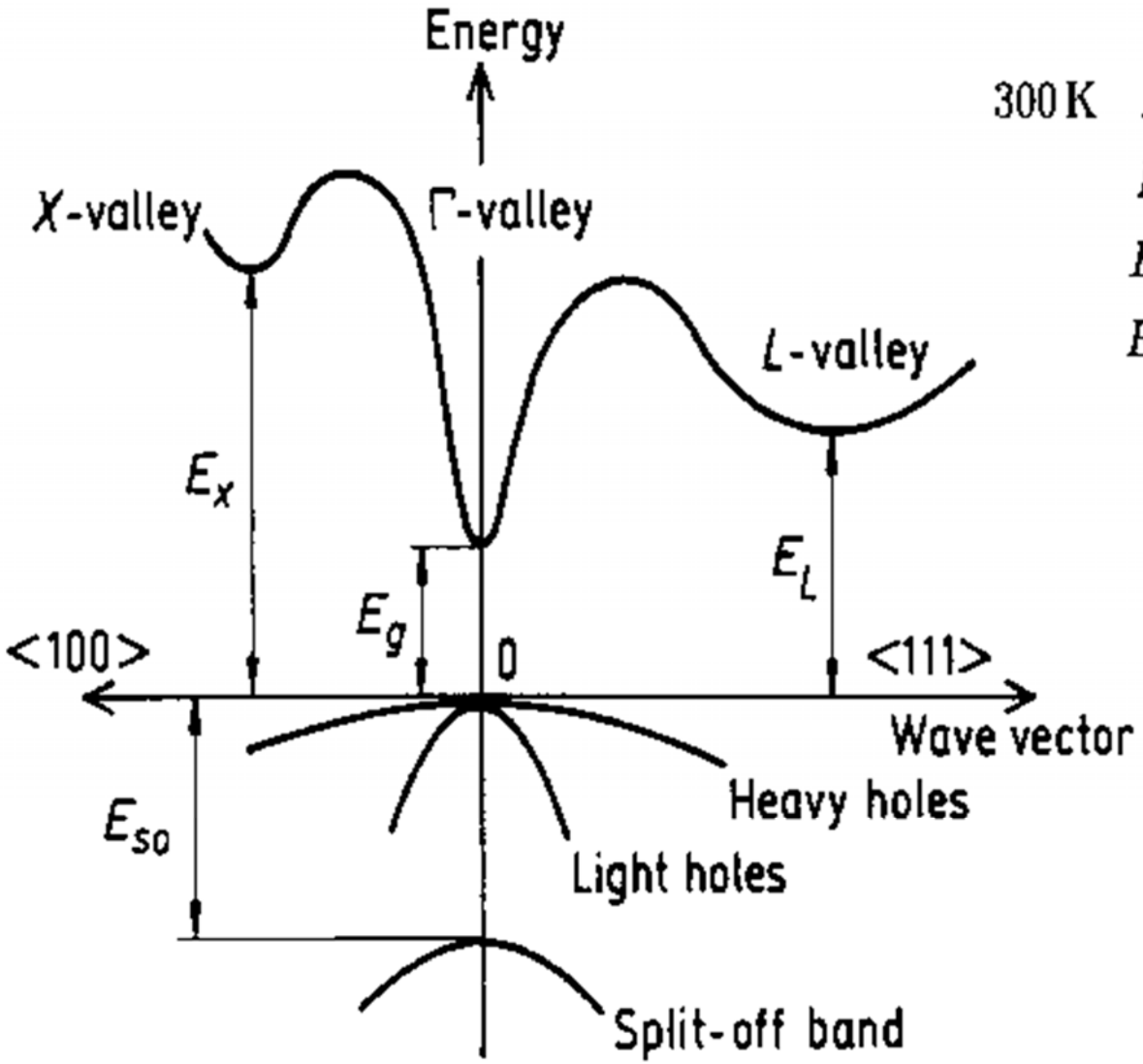
degeneracy 3 * 2 = 4 + 2

this gives
heavy/light hole bands (4)
so-split bands (2) lowered by E_{so}

E_{so} spin-orbit strength ~ local electric field of atom on site ~ nuclear charge Z

Eso ~	6 meV	graphite
	45 meV	Si
	340 meV	GaAs

GaAs band structure



300 K $E_g = 1.42$ eV

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Valence bands (3)

dispersion of the remaining bands
"k·p" approximation (around minima / maxima)

$$\left\{\frac{\hbar^2}{2m}(-i\nabla + k)^2 + U(r)\right\} u_k(r) = \varepsilon_k u_k(r) \qquad (4)$$

write out ( )^2 and replace -i∂ with p (p: operator, k: number)

$$\left[\frac{p^2}{2m} + \frac{\hbar\vec{k}\cdot\vec{p}}{m} + \frac{\hbar^2k^2}{2m} + V(r)\right] u_{n,k}(\vec{r}) = E_{n,k}u_{n,k}(\vec{r})$$

simple
shift

treat k·p term perturbatively….
different masses: light and heavy holes, but degenerate at k=0

hole masses: negative hole charge: negative positive transport (q/m)

Valence bands (4)

hole masses

Si $m^*_{HH} = 0.54\ m_e$

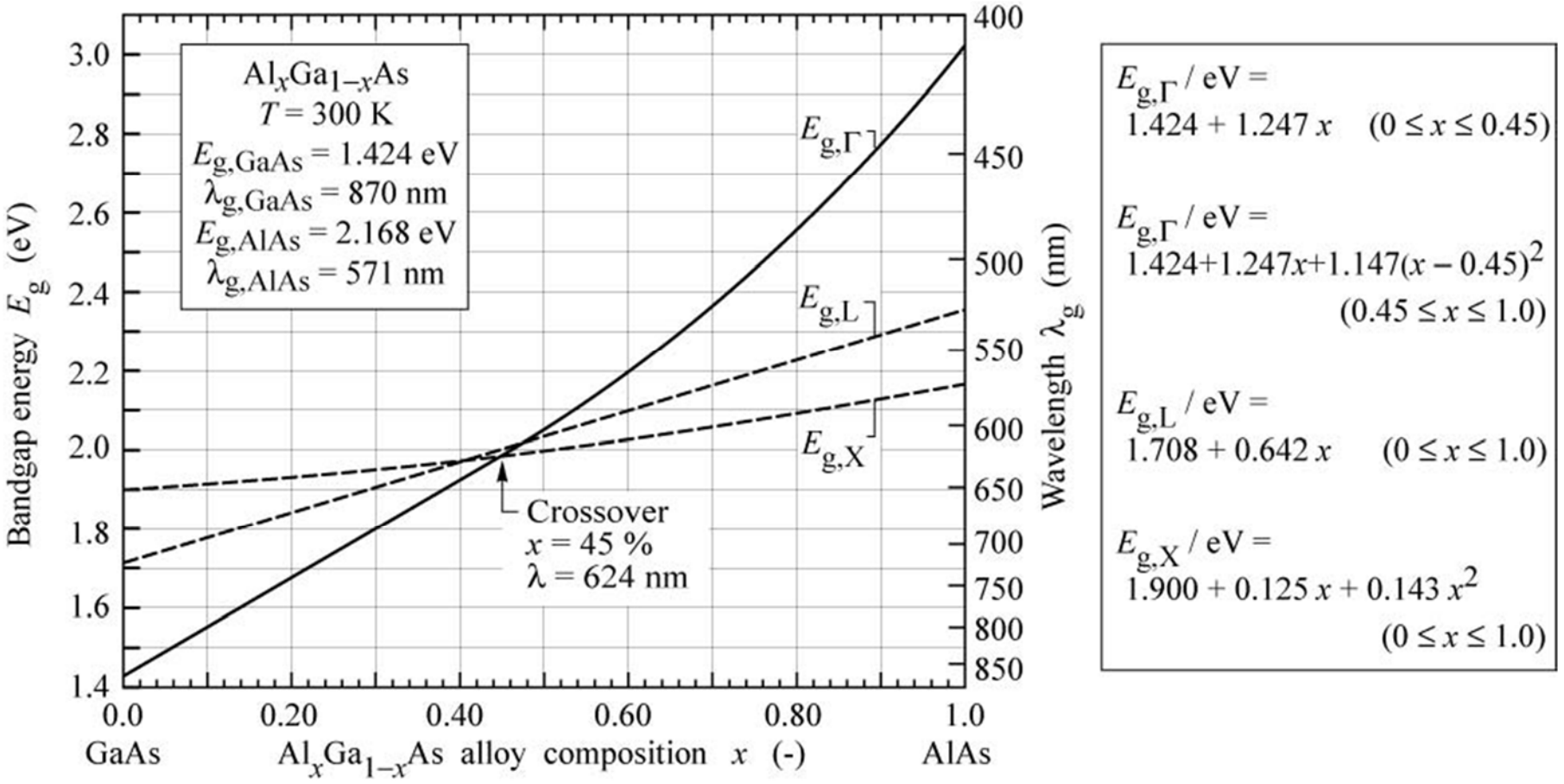
$m^*_{LH} = 0.15\ m_e$

GaAs $m^*_{HH} = 0.51\ m_e$

$m^*_{LH} = 0.08\ m_e$

(vs. GaAs electron mass $0.067\ m_e$)

Replace fraction 0≤x ≤1 with Aluminium (Al): $Al_XGa_{1-X}As$



$E_{g,\Gamma}$ / eV =
$1.424 + 1.247\,x$ $(0 \le x \le 0.45)$

$E_{g,\Gamma}$ / eV =
$1.424+1.247x+1.147(x-0.45)^2$
$(0.45 \le x \le 1.0)$

$E_{g,L}$ / eV =
$1.708 + 0.642\,x$ $(0 \le x \le 1.0)$

$E_{g,X}$ / eV =
$1.900 + 0.125\,x + 0.143\,x^2$
$(0 \le x \le 1.0)$

Fig. 12.7. Bandgap energy and emission wavelength of AlGaAs at room temperature. E_Γ denotes the direct gap at the Γ point and E_L and E_X denote the indirect gap at the L and X point of the Brillouin zone, respectively (adopted from Casey and Panish, 1978).

Occupation of bands

electronic density of states $D_d(E)$

# of states available in a window of energy [E, E+dE].
d : dimensionality of the system

periodic boundary conditions (cube, square, line) of length L
(endresult independent of L)

$$\psi\left(\vec{r} + (L, L)\right) = \psi\left(\vec{r}\right)$$

Electronic Density of States

$$D_1(E) = \frac{g\sqrt{2m}}{2\pi\hbar}\frac{1}{\sqrt{E}}$$

$$D_2(E) = \frac{gm}{2\pi\hbar^2}$$

independent of energy

$$D_3(E) = \frac{g\,(2m)^{3/2}}{4\pi^2\hbar^3}\cdot\sqrt{E}$$

plus Fermi-Dirac distribution gives carrier occupation…

Doping

Control mobile carrier type (n or p) and density by implanting dopants
donors (give off electron) or acceptors (take in electron)

example replace Ga (3 valence electron) with Si (4 valence electrons)
1 extra electron (plus a proton left behind)

similar to a hydrogen atom in a medium with dielectric constant ε_{GaAs} ~ 13

$$\left[-\frac{\hbar^2}{2m^*}\vec{\nabla}^2 - \frac{e^2}{4\pi\epsilon\epsilon_0 r}\right]\psi(r) = [E - E_C]\,\psi(r)$$

(envelope wave function ψ varies slowly compared to unit cell)

$$E_{DOPANT} = E_C - 13.6\,\mathrm{eV}\frac{m^*}{\epsilon^2 m_e} \qquad \frac{m^*}{\epsilon^2 m_e} \sim \frac{1}{2500}$$

binding energy ~ 5.4 meV

Bohr radius: $a_B^* = \epsilon\frac{m}{m_e}a_B \sim 10.3\,\mathrm{nm} \gg 5.4\,\text{Å}$

atomic Bohr radius: 0.53 Å