

# Crystal Structure

Si and GaAs: face centered cubic

Si: two atom base diamond structure  
 $(a/4, a/4, a/4)$  shifted

GaAs: same, but 1 atom: Ga zincblende structure  
 1 atom: As

$a =$  lattice constant  $= 5.65 \text{ \AA}$  Si  
 $5.43 \text{ \AA}$  GaAs

reciprocal lattice: bcc  $\rightarrow$  Brillouin zone,  $\Gamma, X, L$  points etc.

periodic table III IV V

	11 5B	12 6C	14 7N	16 8O
	27 13Al	28 14Si	31 15P	32 16S
65 30Zn	70 31Ga	73 32Ge	75 33As	79 34Se
112 48Cd	115 49In	119 50Sn	122 51Sb	
	204 81Tl	207 82Pb	209 83Bi	
	valence $e^-$ : 3	4	5	

$\rightarrow$  GaAs: III-V compound (binary)

other III-IV  $\rightarrow$  also zinc blende

## Bands

Electrons obey the Schrödinger equation (neglecting interaction)

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

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

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

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

in periodic potential;  $\hookrightarrow$  parabolic dispersion

periodicity, Bloch theorem:

2

$$\psi(r) = \Psi_k(\vec{r}) = e^{ik \cdot r} u_k(r) \quad (2)$$

$$\text{with } u_k(r+R) = u_k(r) \quad (3)$$

put (2) in (1), get

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

with periodic boundary conditions. (3)

→ (4) is eigenvalue problem for finite size/volume resulting in discrete spectrum, called

ENERGY BANDS →  $\epsilon_n(k)$

$k$  is additional (continuous, but limited to 1st Brillouin zone) parameter, i.e.

$$\epsilon_k = \epsilon_{n,k}, \quad \Psi = \Psi_{nk}(r) \quad \text{solution of (4)}$$

→ metals, semicond., insulators.

exact solution usually impossible, various approx. methods exist. result for Si and GaAs (different because Si (free electrons, tight binding, ...) base covalent, GaAs polar)

Si: indirect gap → momentum mismatch for photons  
GaAs: direct gap → ok photons

Effective mass Approx.

expand  $E(\vec{k})$  relation at minima / maximum:

$$E(\vec{k}) = E_0 + \frac{1}{2} \vec{k} \cdot \underbrace{\frac{\partial^2 E}{\partial k_i \partial k_j}}_{\sim m_{ij}^*} \vec{k} \quad (5)$$

$\sim m_{ij}^*$  "effective mass"

→ tensor, symmetric → diagonalize →

three principal eff. masses (along principal axes)

→ carriers behave like free electrons with eff. mass.  
conduction bands not degenerate + spin

Si: minimum / gap X direction  $\sim 0.85 \Gamma$  X  
ellipsoids; anisotropic eff. mass

$$m_{e, \text{transverse}} = 0.19 m$$

$$m_{e, \text{long.}} = 0.92 m$$

Ge: gap @  $\Gamma$  / zero, isotropic mass,  $m^* = 0.067 m$

Valence Band: built from atomic p-states  
→ 3 fold orbital degeneracy + spin

spin-orbit coupling: electric field

$$H_{so} = \frac{\hbar}{4m^2 c^2} \vec{\sigma} \cdot \overbrace{\nabla V}^{\text{electric field}} \wedge \vec{p} \quad (6)$$

$V$  : electrostatic pot.

$\vec{\sigma}$  : Pauli matrix vector

$\vec{p}$  : momentum operator

relativistic effect (follows from Dirac eq.):

(motion in electric field → Lorentz transf. gives magnetic field component, → couples to spin  $\vec{\sigma}$  via Zeeman term)

in spherically symmetric potential  $\rightarrow$

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

$\vec{L}$ : angular momentum  
 $\vec{S}$ : spin

assume we can consider electrons in solid as in an individual atom,  $p \approx \hbar k \rightarrow L=1$ , spin  $S=1/2$

$$\rightarrow 1 \otimes 1/2 = 3/2 \oplus 1/2$$

degeneracy 4      2

$\rightarrow$  understand heavy-light hole (4) + sp-split bands(?) which is split off (lowered) by  $E_{so}$

$E_{so} \sim$  spin orbit strength  $\sim$  local electric field of atom on site  $\sim$  weight of nucleus (stronger for heavier)

$E_{so} \sim$	6 meV	graphite
	45 meV	Si
	340 meV	GaAs

Dispersion of remaining four bands:

k.p approximation, to model dispersion @ extralnd pts

multiply out ( )<sup>2</sup> in (4) writes  $\nabla$  as p

$$(7) \left\{ \frac{p^2}{2m} + \frac{\hbar \vec{k} \cdot \vec{p}}{m} + \frac{\hbar^2 k^2}{2m} + V(r) \right\} u_{n,k}(r) = E_{n,k} u_{n,k}(\vec{r})$$

$\leftarrow$  simple shift  $\rightarrow$  drop

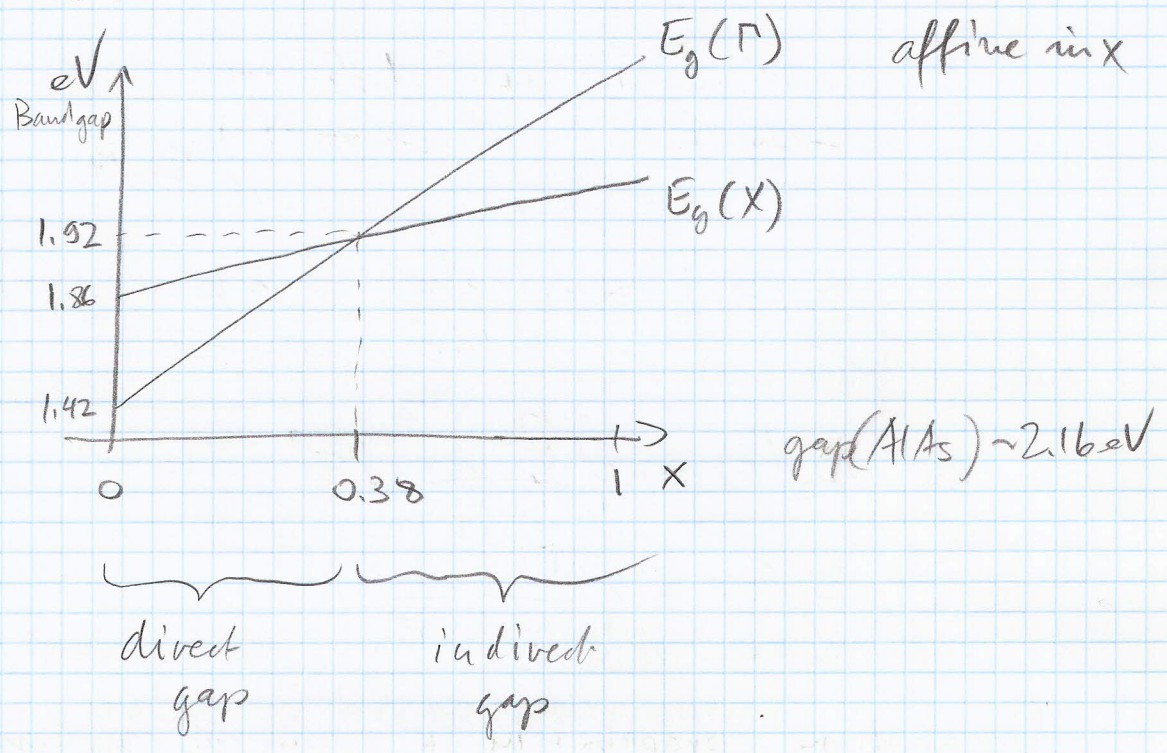
point of interest:  $k=0 \rightarrow$  simplifies (k.p) path treat nonzero k (for dispersion) perturbatively  $\rightarrow$  not shown

heavy + light hole masses, but degenerate at  $k=0$  (only lifted by Dresselhaus term  $\sim \mu eV$ )

hole masses: negative } transport:  $q/m \rightarrow$  positive  
 hole charge: negative }

Si:  $m_{hh}^* = 0.54m$   
 $m_{lh}^* = 0.15m$   
 GaAs:  $m_{hh}^* = 0.51m$   
 $m_{lh}^* = 0.08m$

Often, Al replaces fraction  $x$  of Ga atoms  
 Al<sub>x</sub>Ga<sub>1-x</sub>As (replacement at random loc. → not crystal)



Occupation of Bands

→ per volume/area/length  
 electronic density of states  $D_d(E) = \#$  of states available in energy window  $[E, E+dE]$ .  $d$  is the dimensionality of system.  $D(E)$  also depends on dispersion.

$d=2$

periodic boundary conditions in cube/square of length  $L$  (ends result with not depend on  $L$ )

$\psi(\vec{r} + (L, L)) = \psi(\vec{r})$   $\vec{k} = \frac{2\pi}{L}(n_x, n_y)$

with  $n_x, n_y$  integers. each  $k$  point has degeneracy

$2$  (spin)  $\times$  valley degeneracy  $= g$

number of states in  $k$  space :  $\left(\frac{L}{2\pi}\right)^2$

6

for given  $|\vec{k}|$  :  $g \cdot \underbrace{\pi |\vec{k}|^2}_{\text{circle area}} \cdot \underbrace{\left(\frac{L}{2\pi}\right)^2}_{\text{\# of states}}$  states

$$dN_2 = \# \text{ states in annulus } [|\vec{k}|, |\vec{k}| + dk] \\ = g \left(\frac{L}{2\pi}\right)^2 2\pi |\vec{k}| dk$$

$D_2(k)$  = density of states in  $k$ -space

$$= \frac{1}{L^2} \frac{dN_2}{dk} = \frac{gk}{2\pi}$$

$$E(k) = \frac{\hbar^2 k^2}{2m^*} \quad dE = \frac{\hbar^2}{m^*} k dk \quad \frac{dk}{dE} = \frac{m^*}{\hbar^2 k}$$

$$D_2(E) = D_2(k) \frac{dk}{dE} = \boxed{\frac{g m^*}{2\pi \hbar^2} = D_2(E)} \quad (8) \quad \text{indep. of } E$$

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

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

## Occupation probability + chemical potential

electrons = fermions

equilibrium  $\rightarrow$  Fermi-Dirac distribution

$$f(E, T) = \frac{1}{e^{(E-\mu)/k_B T} + 1} \quad (9)$$

$\mu$  = chemical potential : energy for which DOS occupied = DOS empty

$T$  = temperature

Fermi Energy : Energy where  $f$  goes from 1 to 0 at  $T=0$   
( $\rightarrow \mu = E_F$  at  $T=0$ )

(at  $T > 0$   $\mu \neq E_F$  generally, depending on density of states)

metals:

partly occupied band at  $T=0$   
 $E_F$  in a band

semi cond:  
 (intrinsic = dopant free)  
 perfect

conduction band empty, valence band full  
 at  $T=0$  (cond. b. only thermally populated at  $T \neq 0$ )  
 $E_F$  in gap. (ditto insulators)  
 (roughly equal  $e + h$  pop.)

$n$  = electron density (# of electrons per area) (total)

$n(E)$  = # of electrons up to energy  $E$

$$n = \int_{E_{\text{bottom}}}^{E_{\text{top}}} n(E) dE = \int_{E_{\text{bottom}}}^{E_{\text{top}}} D(E) \cdot f(E, T) dE \quad (10)$$

(dimensionality of  $D(E)$  determines dimensi. of  $n$ , since  $f$  is dimensionless)

## Doping

control predominant type of mobile carrier by implanting donors or acceptors (dopants)

example: replace a Ga with a Si

$\downarrow$   
 3 val.  $e^-$

$\downarrow$   
 4  $e^-$

$\rightarrow$  1  $e^-$  extra

(Si also has 1 nuclear charge left (proton) positive)

like a hydrogen atom in a medium with dielectric constant  $\epsilon \approx 13 \rightarrow$  Schrödinger Eq.

$$\left\{ -\frac{\hbar^2}{2m^*} \Delta - \frac{e^2}{4\pi\epsilon\epsilon_0 r} \right\} \psi(r) = [E - E_c] \psi(r) \quad (11)$$

(envelope wave function approx:  $\psi(r)$  varies slowly comp. to unit cell)

$$E_{\text{Dopant}} = E_c - \underbrace{13.6 \text{ eV}}_{R_y} \cdot \frac{1}{f^2} \frac{1}{\epsilon^2} \frac{m^*}{m_e}$$

$$\frac{1}{\epsilon^2} \frac{m^*}{m} \sim 2500 \rightarrow \text{binding energy} \sim 5.4 \text{ meV}$$

Bohr radius  $a_B^* = \epsilon \frac{m}{m^*} a_B \approx 0.3 \text{ nm} \gg 5.4 \text{ \AA}$  lattice const.

intrinsic carrier concentration

thermal excitation of electrons from valence to conduction band only  $\rightarrow n = p$

$$n = \frac{\sqrt{2} m_e^{*3/2}}{\pi^2 \hbar^3} \int_{E_c}^{\infty} \sqrt{E - E_c} f(E, T) dE \quad (12)$$

el. density ↑      ↑ hole density

$$p = \frac{\sqrt{2} m_h^{*3/2}}{\pi^2 \hbar^3} \int_{-\infty}^{E_v} \sqrt{E_v - E} f(E, T) dE \quad (13)$$

only difference: effective masses: heavier  $\rightarrow$  more states  
 chemical potential  $\mu \rightarrow$  slightly shifted from center to lighter mass band  
 (fixed by  $n=p$ )

usually  $m_n \sim m_e$  within small factor

$|E_{c,v} - \mu| \gg k_B T \rightarrow$  keep only tails of FD distr. in valence/cond band  
 $\rightarrow$  Boltzmann exponential

do integrals - (use  $\Gamma$ -fact.  $\int_0^{\infty} \sqrt{x} e^{-x} dx = \sqrt{\pi}$ )

$$n = N_c e^{-(E_c - \mu)/kT} \quad p = P_v e^{-(E_v - \mu)/kT} \quad (14)$$

$$N_c = \frac{1}{4} \left( \frac{2m_e^* kT}{\pi \hbar^2} \right)^{3/2} \quad P_v = \frac{1}{4} \left( \frac{2m_h^* kT}{\pi \hbar^2} \right)^{3/2}$$

notice  $n \cdot p = N_c P_v e^{-E_g/kT} \rightarrow \boxed{n=p = \sqrt{N_c P_v} e^{-E_g/2kT}}$   
 $(E_g = E_c - E_v)$  (15)



this also fixes  $\mu$ , by inserting into (14)

$$\mu = E_V + \frac{1}{2} E_g + \frac{3}{4} kT \ln\left(\frac{m_{lh}^*}{m_{le}^*}\right) \quad (16)$$

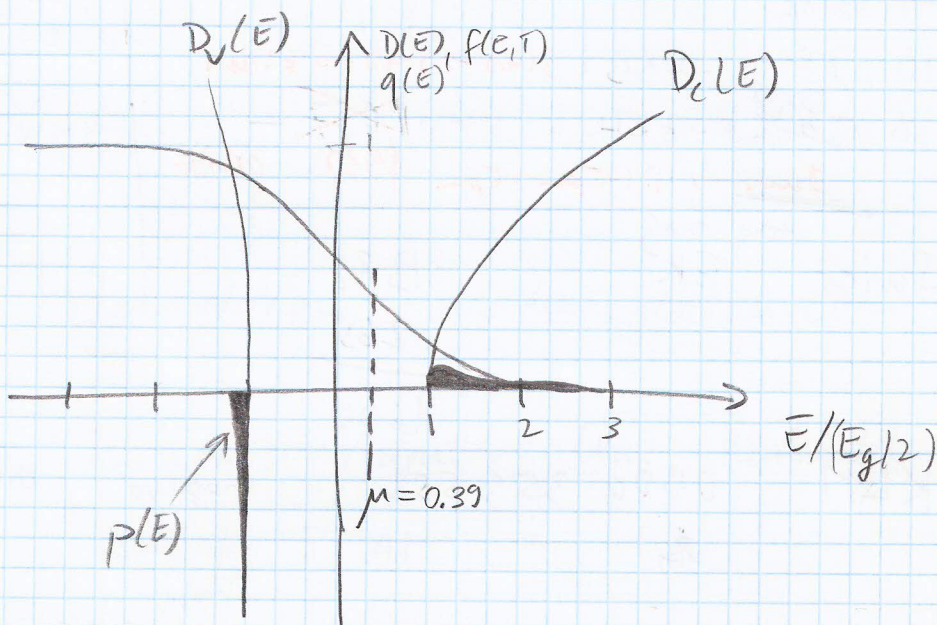
$kT \ll E_g$  carrier freezeout

room T:

$$n_{Si} = 1.45 \cdot 10^{16} \text{ m}^{-3}$$

$$n_{GaAs} = 1.8 \cdot 10^{12} \text{ m}^{-3}$$

} "small"  
(compared to  $N_{AVO} (10^{23})$ )



for  $m_n^* = 2 m_e^*$  (GaAs  $m_{hh}^* \sim 10 m_e^*$ )

- full or empty bands: no current
- resistance of at least one partially filled band zero  
resistance in real materials from defects, phonons, dislocations  
surface/interface etc (but not usually from  $e^-e^-$  scattering)