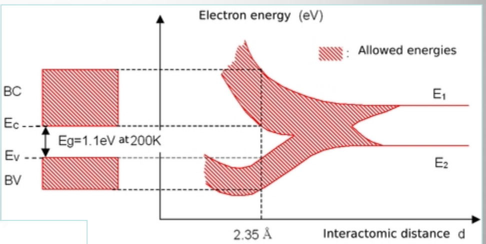
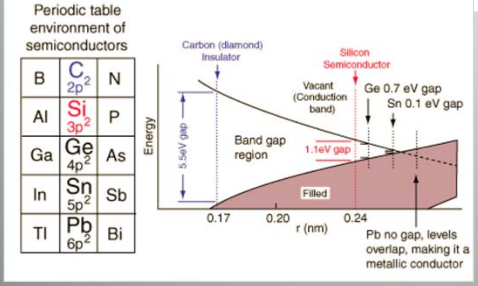
Dr. Gregory W. Clark
Manchester University

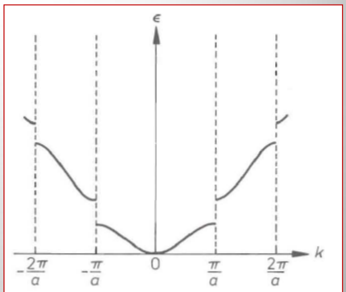




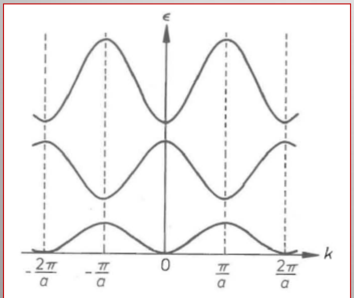
PHYS432
Materials Physics

Band Structure

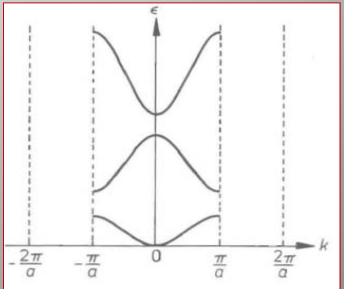
- Visualizing the gaps



Extended zone scheme



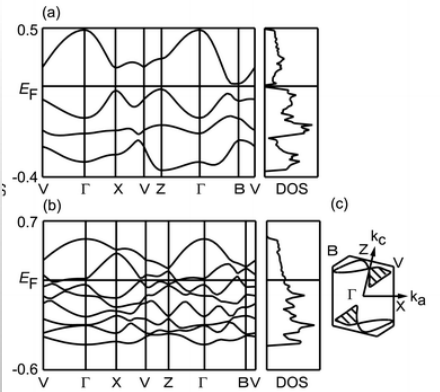
Repeated zone scheme

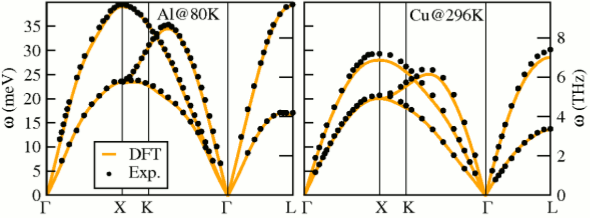


Reduced zone scheme

Band Structure

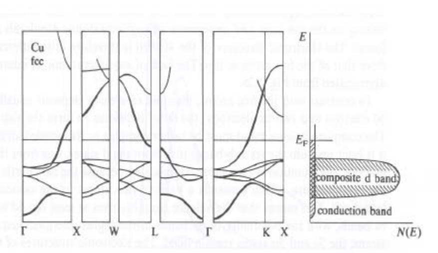
- See text!
- P. 88

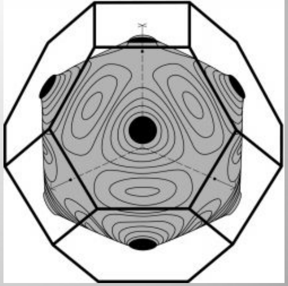


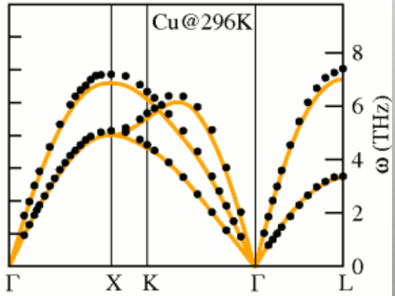


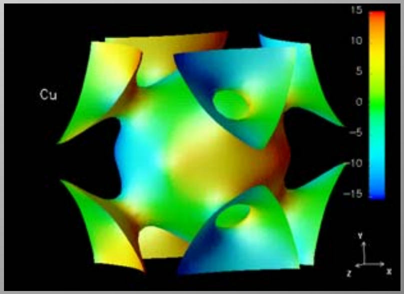
Fermi Surface

- Copper









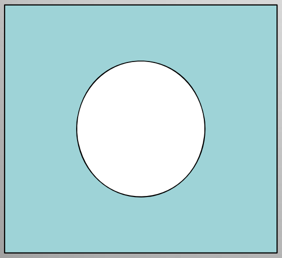
Quasi-Particles

- "Free" electron in Xtal: $\left\{ \begin{array}{l} E_n \\ q_n = -e \\ m_n^* \\ \vec{k}_n \end{array} \right.$
- Holes in Xtal: $\left\{ \begin{array}{l} E_p = -E_n, \\ q_p = -q_n = e \\ m_p^* = -m_n^* \\ \vec{k}_p = -\vec{k}_n \end{array} \right.$
- Excitons (e^-/h^+ bound states)

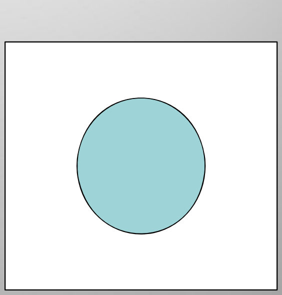
Quasi-particles behave as if "free" and have effective mass m^* in external force (internal forces compensated by m^*)

Holes

- Occupied states in k-space: two equivalent views (*e.g.*, Na, spherical FS)



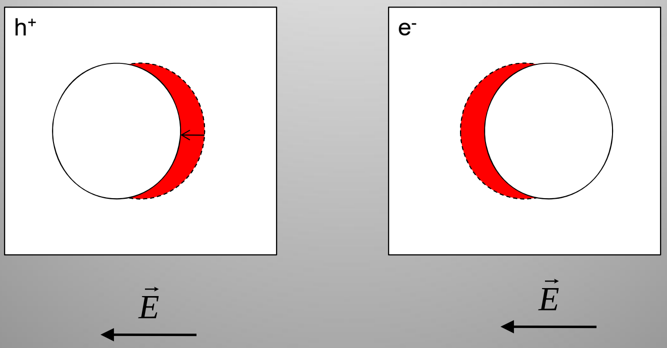
h^+ filled states outside FS



e^- filled states inside FS

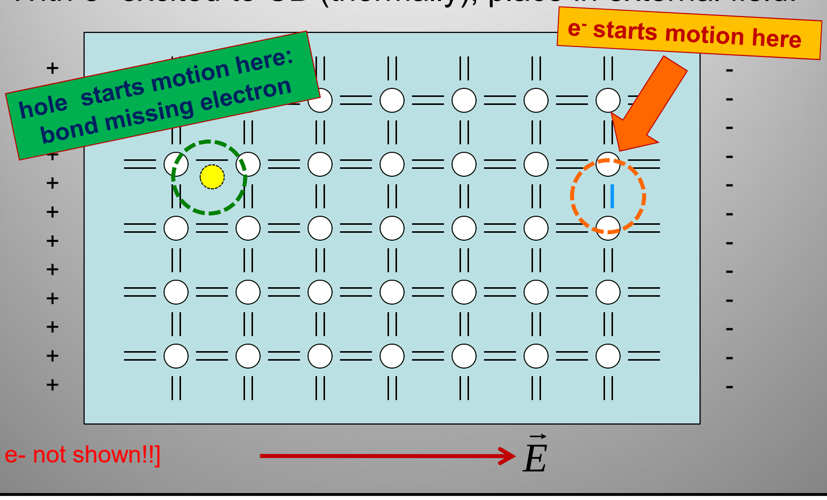
Holes in an electric field

- FS displaced in direction of field for holes, opposite direction for electrons
- Results in uncompensated h^+ or e^-



Visualizing holes: covalent Xtal: Si

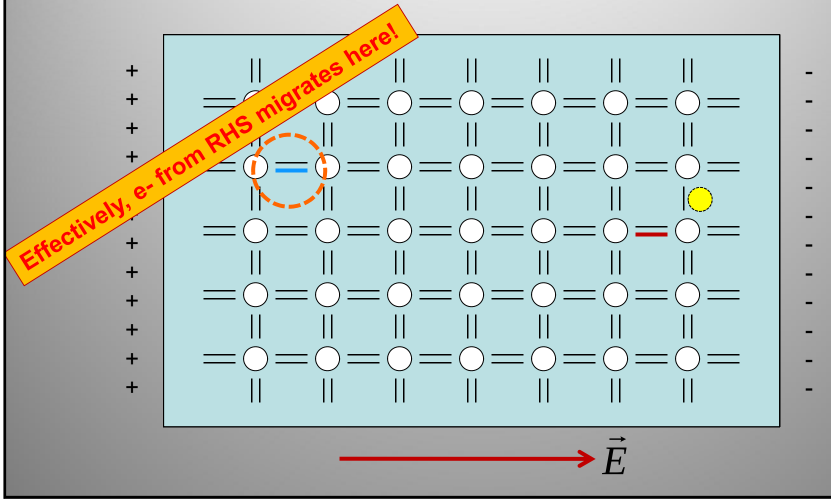
- Just enough **valence** states to accommodate all the e^- involved in covalent bonds with neighbors.
- With e- excited to CB (thermally), place in external field:



[CB e- not shown!!]

Visualizing holes: covalent Xtal: C or Si

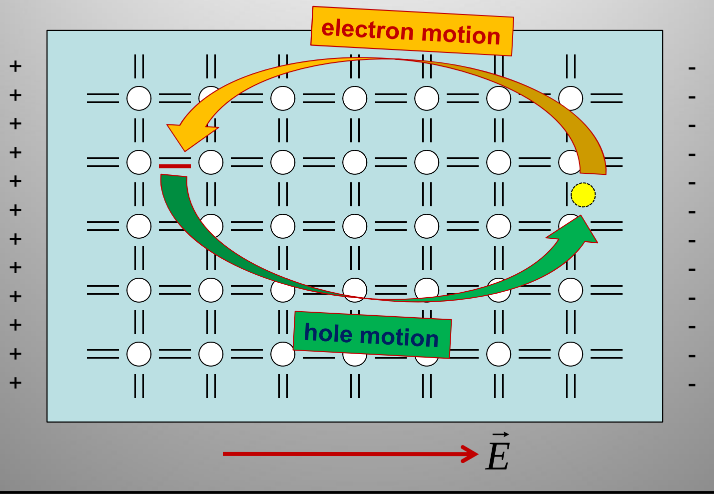
- Hole migrates toward negative side
- Electron migrates toward positive side



E.g. covalent Xtal: C or Si

Net effect: e^- move in one direction; holes move in opposite

$\sigma = |e|(n\mu_e + p\mu_h)$ where μ = mobility, n & p are concentrations



Semiconductors

Crystal lattice
real and reciprocal space

Structure of Silicon;
Germanium

Band theory of solids

Fermi energy;
Effective mass;
Energy gap;
Density of states;
Fermi distribution

Semiconductors

MS junction

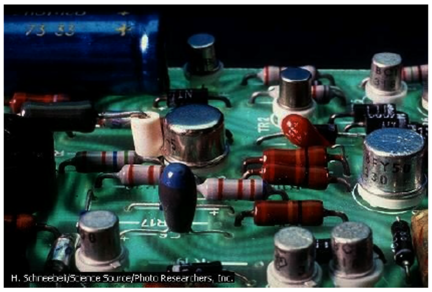
Transistor

p-n
junction

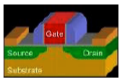
Structure

Intrinsic
semiconductor

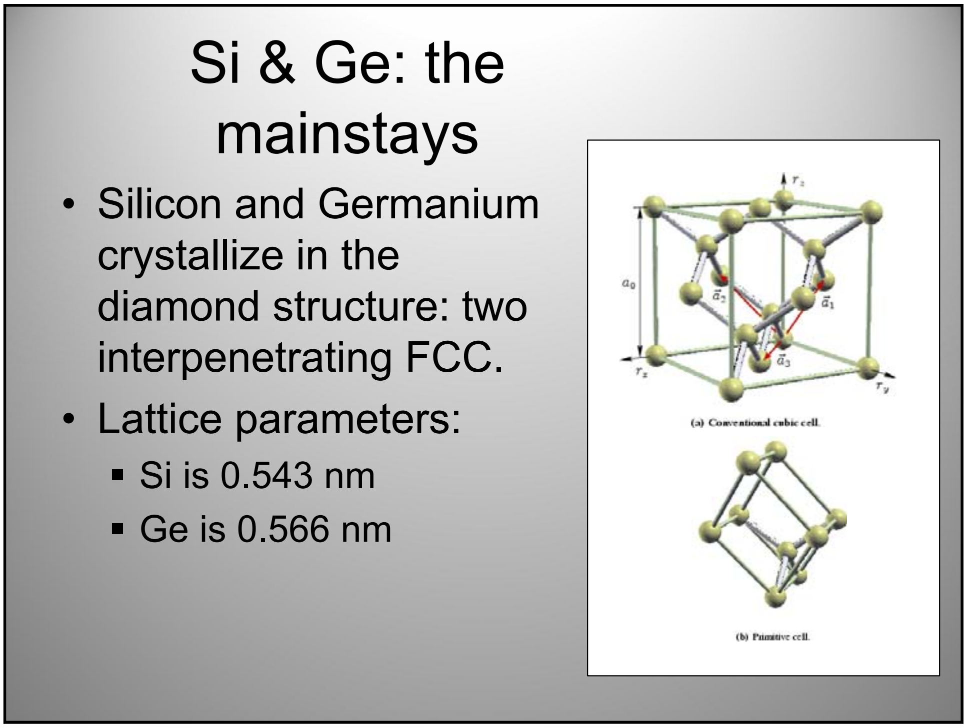
Doped
semiconductor


H. Schneebeli/Science Source/Photo Researchers, Inc.

FET
Mos-FET



Laser
diode

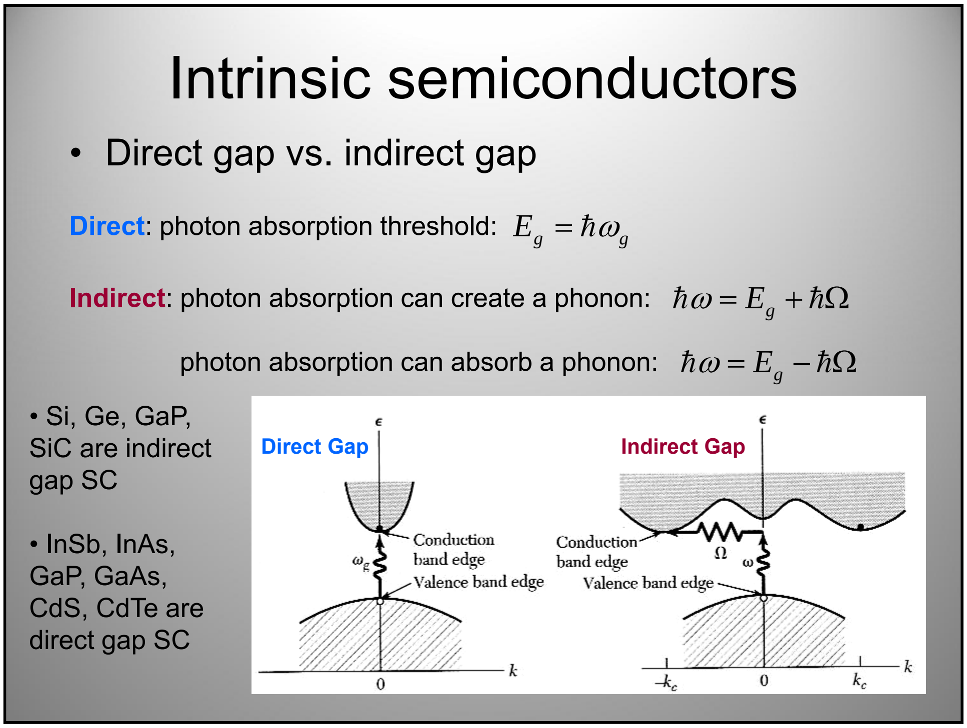


Si & Ge: the mainstays

- Silicon and Germanium crystallize in the diamond structure: two interpenetrating FCC.
- Lattice parameters:
  - Si is 0.543 nm
  - Ge is 0.566 nm

(a) Conventional cubic cell.

(b) Primitive cell.



Intrinsic semiconductors

- Direct gap vs. indirect gap

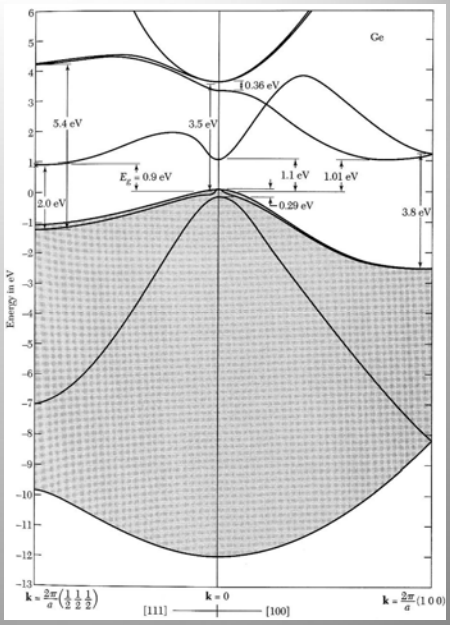
Direct: photon absorption threshold: $E_g = \hbar\omega_g$

Indirect: photon absorption can create a phonon: $\hbar\omega = E_g + \hbar\Omega$

photon absorption can absorb a phonon: $\hbar\omega = E_g - \hbar\Omega$

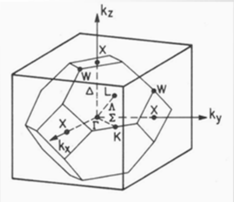
- Si, Ge, GaP, SiC are indirect gap SC
- InSb, InAs, GaP, GaAs, CdS, CdTe are direct gap SC

Ge band structure

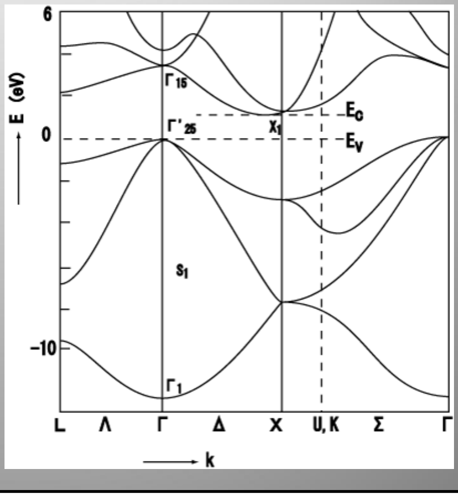


Semiconductors

- Si band structure: indirect gap

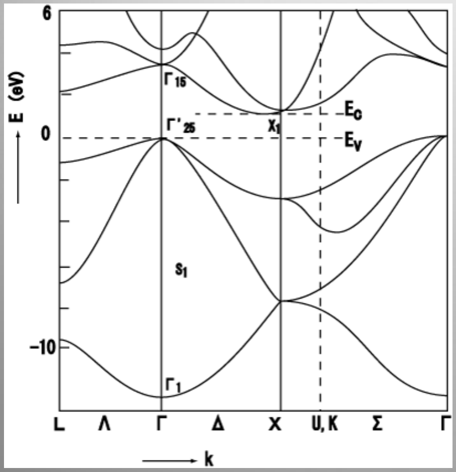


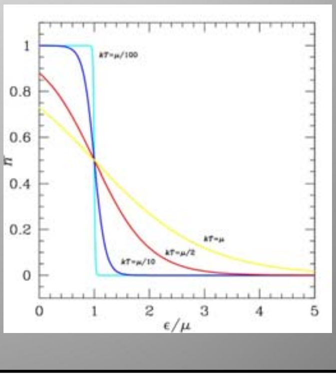
	E_g (eV)
InSn	0.18
InAs	0.36
Ge	0.67
Si	1.11
GaAs	1.43
SiC	2.3
ZnS	3.6
C (dia)	5.5



- http://jas.eng.buffalo.edu/education/semicon/fermi/levelAndDOS/index.html

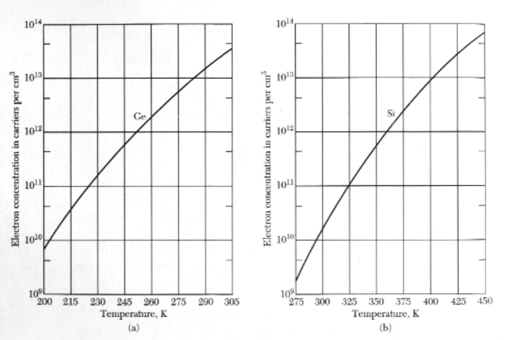
Si Structure

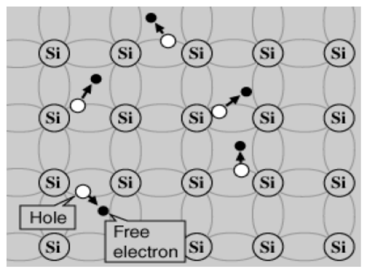


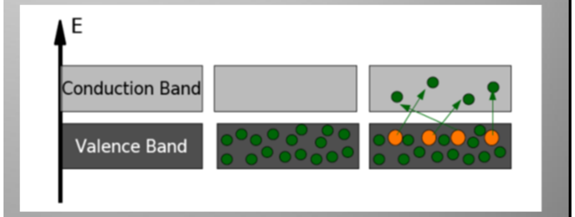


Intrinsic Semiconductors

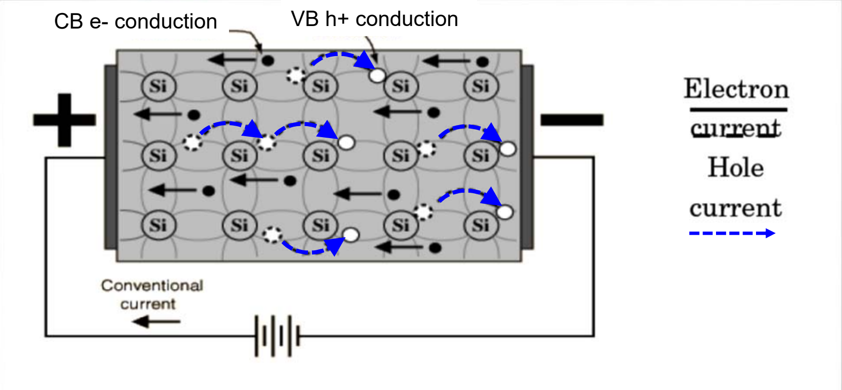
- E_g small enough that some e- excited to CB at RT
- h+ created in VB







Intrinsic semiconductors

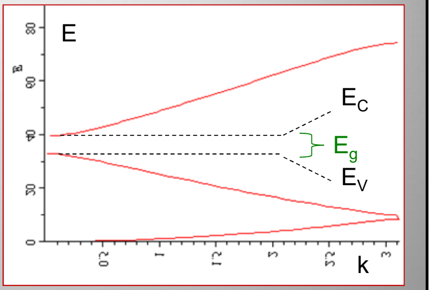


Current in intrinsic semiconductor consists of both e- and h+ current:

$\sigma = |e|(n\mu_e + p\mu_h)$, where μ_e and μ_h = electron & hole mobility, respectively and n and p = electron & hole concentrations, respectively

Density of Occupied/Unoccupied States

- Build on what we know: simple model
- Think Kronig-Penney-like

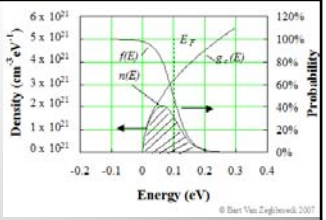


- Consider points in 2nd (=VB) and 3rd (=CB) bands, at k ~ 0
- VB is hole-like: m* < 0
- CB is e⁻-like: m* > 0

Free-electron-like model using effective masses

$$E = \frac{\hbar^2 k^2}{2m^*}$$

Density of Occupied/Unoccupied States



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* Free-electron-like model using effective masses

$$DOS = g_{CB}(E)\,f_D(E) = \left(\frac{V}{2\pi^2}\right)\left(\frac{2m_n^*}{\hbar^2}\right)^{\frac{3}{2}}(E-E_C)^{\frac{1}{2}}[1+e^{(E-E_F)/k_BT}]^{-1}$$

$$DUS = g_{VB}(E)[1-f_D(E)] = \left(\frac{V}{2\pi^2}\right)\left(\frac{2m_p^*}{\hbar^2}\right)^{\frac{3}{2}}(E_V-E)^{\frac{1}{2}}\{1-[1+e^{(E-E_F)/k_BT}]^{-1}\}$$

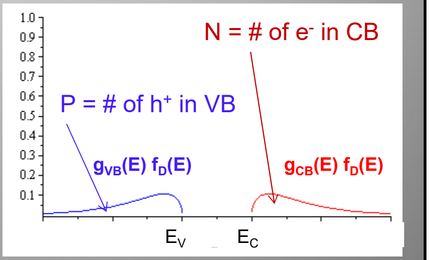
* Area under curves is same for intrinsic semiconductors:

∴ n = density of e^- in CB

= p = density of h+ in VB:

$$n = \frac{N}{V} = \frac{1}{V}\int_{E_C}^{\infty}(DOS)dE$$

$$= p = \frac{P}{V} = \frac{1}{V}\int_{0}^{E_V}(DUS)dE$$



Density of Occupied/Unoccupied States

- At low T (*i.e.*, RT), approximate $f_D(E)$ by the Maxwell-Boltzman distribution function ("non-degenerate" SC):

$$f(E) = e^{-(E-E_F)/k_BT}$$

- The densities become (can actually do the integrals!)

$$n = \left(\frac{\sqrt{2}\,m_n^* k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} e^{-(E_C-E_F)/k_BT} = N_C\, e^{-(E_C-E_F)/k_BT}$$

in the conduction band,
where N_C = **"effective" DOS in the CB**

$$p = \left(\frac{\sqrt{2}\,m_p^* k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} e^{-(E_F-E)/k_BT} = N_V\, e^{-(E_F-E_V)/k_BT}$$

in the valence band,
where N_V = **"effective" DOS in the VB**

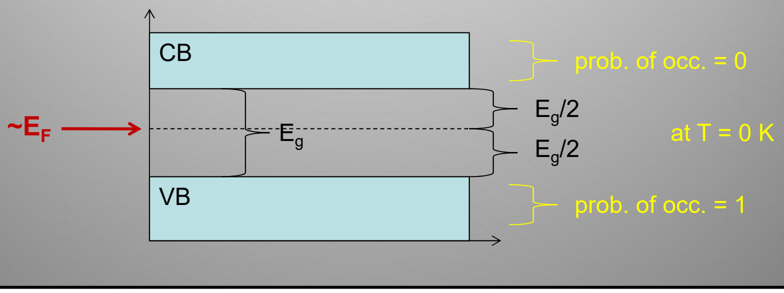
NOTE: These results are valid for intrinsic AND extrinsic (doped) SC!!

e.g., $N_C \sim 10^{25}\ m^{-3}$ @ RT,
so n ~ $10^{16}\ m^{-3}$ for Si @ RT

Semiconductors: Fermi energy?

- E_F = energy for which the probability of occupation is ½ (= chemical potential, μ)
- For metals, E_F approx. constant for *0 K < T < RT*
- Ambiguity when apply to semiconductors
- *"Common sense"* placement of E_F for SC:

  half-way across the gap (good approx. in most circs!)



Density of States

- Must have n = p for intrinsic (pure) semiconductors
- This implies that the "Fermi level" (chem pot'l) is

$$\mu(=\text{"}E_F\text{"}) = \frac{1}{2}(E_C + E_V) + \frac{1}{2}k_B T \ln(N_V / N_C)$$

- EX: For Si: c.p. to metals? n ~ ?? $\boxed{n \sim 10^{28}\ \mathrm{m}^{-3}}$
  - At T = 300 K, $N_C \sim N_V \sim 3 \times 10^{25}\ \mathrm{m}^{-3}$

    >>> $n_i = p_i \sim 10^{16}\ \mathrm{m}^{-3}$
  - At T = 373 K, $n_i = p_i \sim 10^{18}\ \mathrm{m}^{-3}$ (100-fold increase!)
  - $\mu(=\text{"}E_F\text{"}) \approx \frac{1}{2}(E_C + E_V)$ (as we assumed early on)

Density of States

- At T near RT,

$$\mu(="E_F") \approx \frac{1}{2}(E_C + E_V)$$ *(as we assumed early on)*

- So we can approximate the densities as

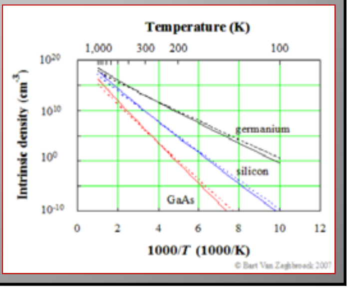
$$n_i = p_i = \sqrt{N_C N_V}\, e^{-E_g/2k_BT}$$

(subscripts can be used for intrinsic!)

- Hence, the law of mass action (intrinsic SC)

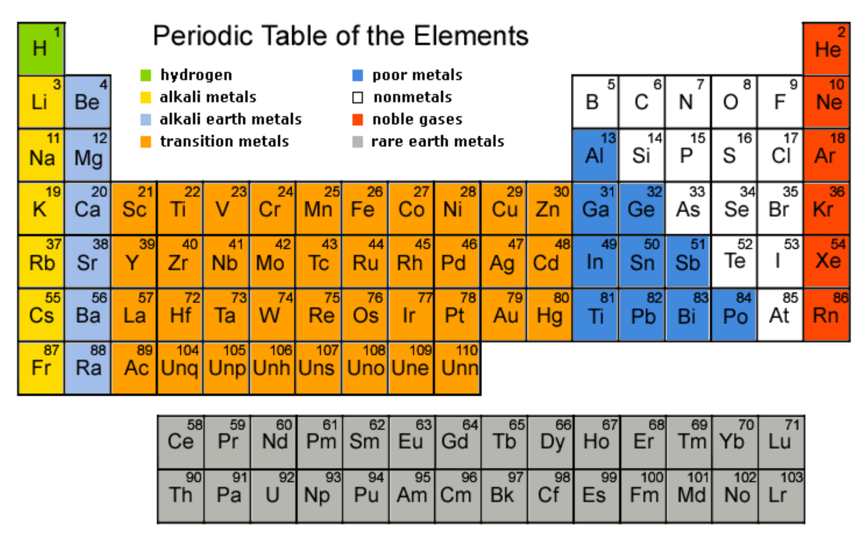
$$n_i^2 = n_i p_i = N_C N_V e^{-E_g/k_BT}$$

(rate of a reaction ~ product of masses of reactants near equilibrium)



Doping

- To increase the number of carriers we can dope the semiconductor, using appropriate impurities that have more/fewer e$^-$ than the intrinsic SC.
- Impurities that contribute electrons to the conduction band are called **donors**.
- Impurities that contribute holes to the valence band are called **acceptors**.
- If a semiconductor contains both donors and acceptors it is called compensated, potentially yielding no free carriers.



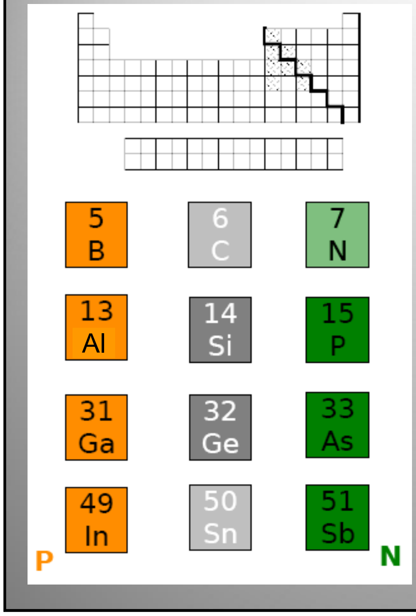
Periodic Table of the Elements

🟩 hydrogen
🟨 alkali metals
🟦 alkali earth metals
🟧 transition metals
🟦 poor metals
☐ nonmetals
🟥 noble gases
⬜ rare earth metals

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Ti	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Unq	105 Unp	106 Unh	107 Uns	108 Uno	109 Une	110 Unn								

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Consider the Periodic Table



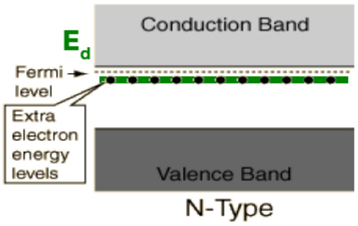
5 B	6 C	7 N
13 Al	14 Si	15 P
31 Ga	32 Ge	33 As
49 In	50 Sn	51 Sb

Conductivity of semiconductors can be modified by addition of impurities. The process of adding impurities is called **doping** and the impurities are called **dopants**.

Two types: **n-type** and **p-type**

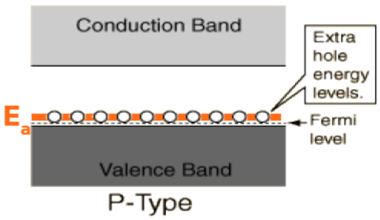
Si must be very pure (and defect-free!) due to extreme sensitivity to impurities (99.9999% pure).

n-type and p-type



In an **n-type semiconductor**, the dopant contributes extra electrons

electrons are said to be the "majority carriers" for current flow in an n-type semiconductor.



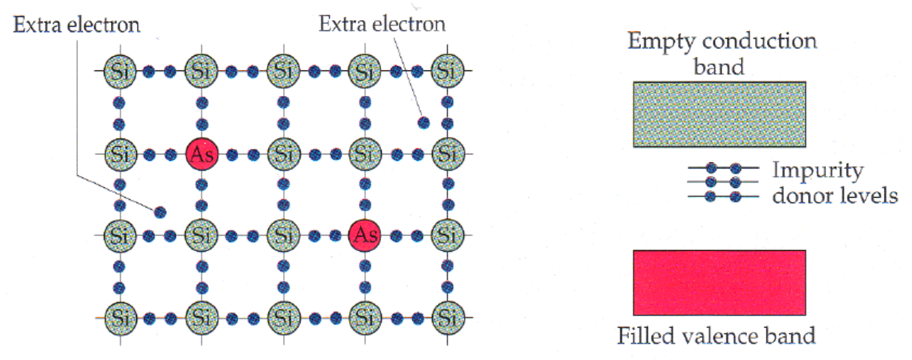
In an **p-type semiconductor**, the dopant contributes extra holes

holes are said to be the "majority carriers" for current flow in an p-type semiconductor.

n-type semiconductors

- **Donor** atoms

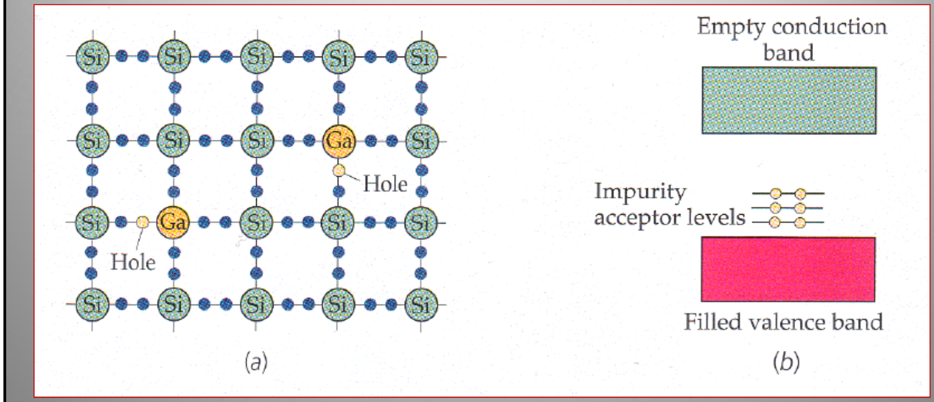
majority carriers: electrons
minority carriers: holes



p-type semiconductors

- **Acceptor** atoms

majority carriers: holes
minority carriers: electrons



p-n junction

- Consists of two semiconducting regions of opposite type with a common interface
- Many technological apps:
  - rectification, isolation, V-dependent capacitor
  - solar cells, photodiodes, light emitting diodes (LEDs), laser diodes
  - Basic element of bipolar junction transistors (BJTs) and field effect transistors (FETs)