Semiconductors

- materials: insulators, semiconductors, conductors
- semiconductors: elemental and compound, direct and indirect
- atom arrangement: single crystal vs. amorphous or polycrystaline
- crystal lattice describes spatial arrangement of atoms: diamond (Si, Ge) or zync-blende (GaAs)
- nature of the bonds between atoms determines band structure: mostly covalent and some ionic (GaAs)

Band Structure

- single atom: allowed electron energies discretized
- lattice: each energy level becomes a band of energies allowed = band structure
- some energies are not allowed = formation of band-gaps
- in semiconductors valence band filled up to the top
- electron bound to atom = no conduction

- thermal excitation breaks up bonds resulting in electron-hole pairs and (small) conduction
- free-electron vs. conduction electron

$$E = \frac{p^2}{2m_0} \qquad\qquad E = \frac{\bar{p}^2}{2m_n} \tag{1}$$

- effective mass analogous to free electron mass

$$m_n = \left(\frac{d^2E}{d\bar{p}^2}\right)^{-1} \tag{2}$$

- crystal momentum analogous to particle momentum
- E vs. $\bar{p}$ = band structure — crucial for understanding semiconductors
- real semic. have more complex band structure: direct vs. indirect cases

Carrier Concentration

- density of states = number of allowed energy states per unit volume in the crystal momentum space

$$N(E) = 4\pi \left[\frac{2m_n}{h^2}^{3/2}\right] E^{1/2} \tag{3}$$

- probabilty that an energy level is occupied — **Fermi-Dirac distribution function**

$$F(E) = \frac{1}{1 + e^{(E-E_F)/kT}} \tag{4}$$

- **Fermi level** = occupation probability 1/2
- simplification: Boltzmann distr. function
- carrier concentration

$$n = \int_0^{E_{top}} N(E)F(E)dE \tag{5}$$

Doping

- intrinsic concentration in the absence of dopants
- derive expression for n_i and justify the assumptions
- impurities (donors or acceptors) introduce additional energy levels near the band edges
- carrier concentration becomes **extrinsic**: n-type from donors, p-type from acceptors
- E_F shifts away from E_i so that

$$n = n_i exp\left(\frac{E_F - E_i}{kT}\right) \tag{6}$$

- without doping there is no electronics!

Drift and Diffusion

- even in equilibrium there is random motion of particles
- average thermal energy of electrons: 1/2 kT per "degree of freedom"; for 3-D system: 3/2 kT
- associated thermal velocity $mv_{th}^2/2 = 3kT/2 \rightarrow v \approx 10^7 cm/s$
- what's stopping these electrons? Collisions, but with what?
- random displacements of lattice atoms, impurities
- mechanism is known as "scattering" (illustrate)
- average distance between collisions — mean free path

- or, mean free time (τ_c) for average time between collisions
- from v_{th} and mean free path l, we can estimate $\tau_c = l/v_{th}$. (example)
- El. field E produces non-equilibrium situation. Some small <u>net</u> drift velocity appears (illustrate)
- The force produced by E on a charge q is $F = -qE$
- force · time = m · v (momentum)

$$-qE\tau_c = mv \rightarrow v = -\frac{q\tau_c}{m}E \tag{7}$$

- v is proportional to E (Ohms law)
- define $\mu = q\tau_c/m$, so that $v = -\mu E$
- since $J = -qnv$, we obtain $J = qn\mu_n E$ which is the <u>drift component</u> of current density J

- drift is not the only mechanism that contributes to conduction — consider diffusion
- diffusion is associated with concentration gradients, i.e., carriers tend to move from the area of high concentration into the lower concentration areas
- simple derivation
- final result for total current density (1-D):

$$J = q\mu_n nE + qD_n \frac{dn}{dx} \tag{8}$$

Carrier Concentrations

- parabolic, isotropic bands $\rightarrow$ density of states

$$\rho_c(E) = \frac{4\pi(2m_n^*)^{3/2}}{h^3}\sqrt{E - E_c} \tag{9}$$

- bandgap $E_g = E_c - E_v$ depends on temperature (inversely) and material
- different effective masses: density-of-state and mobility; dependent on band structure and temperature
- to get concentration some integrating needs to be done
- definition of eff. mass (tensor) relates acceleration and force (due to applied field) — also known as eq. of motion:

$$\frac{1}{m_{ij}} = \frac{1}{m_{ji}} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j} \tag{10}$$

- electron concentration: $n = \int_{E_c}^{\infty} \rho_c f_n(E) dE$ (11)

  where $f_n(E)$ is probability that an energy level E is occupied and is given by Fermi-Dirac distribution

$$f_n(E) = \left(1 + exp\left(\frac{E - E_{fn}}{kT}\right)\right)^{-1} \tag{12}$$

  where E_{fn} is quasi-Fermi level for electrons

- final expression: $n = N_c \frac{2}{\sqrt{\pi}} F_{1/2}\left(\frac{E_{fn} - E_c}{kT}\right)$ (13)

  where N_c is effective density of states (a constant) and $F_{1/2}$ is Fermi integral of order 1/2 (no closed form solution)

1. mention expressions for holes: $E - E_{fn}$ replaced by $E_{fp} - E$
2. Fermi-level is equilibrium concept; also, $E_{fn} = E_{fp}$ in equilibrium
3. Fermi integral: $$F_{1/2} = \int_0^\infty \frac{\sqrt{y}}{1 + e^{y-x}} dy \tag{14}$$
4. no solution causes big problems: many different approx. used
5. often cast into Boltzman-like expression (correction factors etc.)

- Eff. density of states: $$N_c = 2\left(\frac{2\pi kTm_n^*}{h^2}\right)^{3/2} \tag{15}$$

  same for N_v

- by assuming $E_{fn} - E_c \ll -kT$

$$n = N_c exp\left(\frac{E_{fn} - E_c}{kT}\right) \tag{16}$$

- what are all those energies?

- break up E_c and E_v

$$E_c = E_{co} - \delta E_c - q\psi \qquad E_v = E_{vo} + \delta E_v - q\psi \tag{17}$$

E_{co}, E_{vo} are band edges for pure material, δ's are for compositional changes, ψ is electrostatic potential (from Poisson's equation)

- for Fermi levels we have

$$E_{fn} = E_i - q\phi_n \qquad\qquad E_{fp} = E_i - q\phi_p \tag{18}$$

where E_i is Fermi energy for reference intrinsic material, and ϕ_n, ϕ_p are quasi-Fermi potentials.

- arbitrary separation — show illustrations; the end justfies the means

$$n = N_c exp\left(\frac{E_i - E_{co} + \delta E_{co}}{kT}\right) exp\left(\frac{q\left(\psi - \phi_n\right)}{kT}\right) \tag{19}$$

In bulk homogeneous semiconductor we have charge neutrality condition, i.e., $p - n + N_D^+ - N_A^- = 0$. For "pure" material (no doping) $p = n$

Choice of ϕ_n and ψ: set $\phi_n = 0$ for any equilibrium situation (no external forces, or fields). What about ψ? Arbitrary, but choose $\psi = 0$ for pure material. In that case E_i corresponds to Fermi level for "pure" (intrinsic) material.

$$E_i - E_c = \frac{kT}{2} ln\left(\frac{N_v}{N_c}\right) - \frac{E_g}{2} \tag{20}$$

For most semiconductors E_i will be very close to mid-bandgap since effective densities of state for conduction and valance bands are "close"

One additional quantity: intrinsic concentration $n_i = \sqrt{np}$

- valid for both intrinsic ("pure") as well as extrinsic (doped) cases
- easily shown that $n_i = \sqrt{N_c N_v} exp(-E_g/(2kT))$ — material parameters only! Can be position dependent.
- useful for re-writing the concentrations:

$$n = n_i exp\left(\frac{\psi - \phi_n}{U_T}\right) \quad p = n_i exp\left(\frac{\phi_p - \psi}{U_T}\right) \tag{21}$$

where $U_T = kT/q$

What happens to ψ in the extrinsic case? How do we calculate it?

- charge neutrality still assumed

$$n_i exp(-\psi/U_T) - n_i exp(\psi/U_T) + N_D^+ - N_A^- = 0 \tag{22}$$

- usually one doping is much higher than the other making it possible to calculate the ψ — often called built-in potential

$$\psi_b \approx U_T ln(N_D^+/n_i) \tag{23}$$

- without Boltzmann approximation things are more complicated!
- parabolicity and rigid band shifts assumed — what about changes in eff. density of states?