Outline

- Need to know how many carriers at what energy and where in the device
- Properties of Semiconductors
  - Band gap & band diagrams
  - Density of states
  - Fermi-levels
  - Carrier Concentration: Intrinsic and doped
  - Transport properties and mechanisms
  - Recombination and Generation
- PN junctions
  - Built-in electric field
  - Current flow mechanisms under voltage and light bias
  - Diode equation

Energy of Electrons

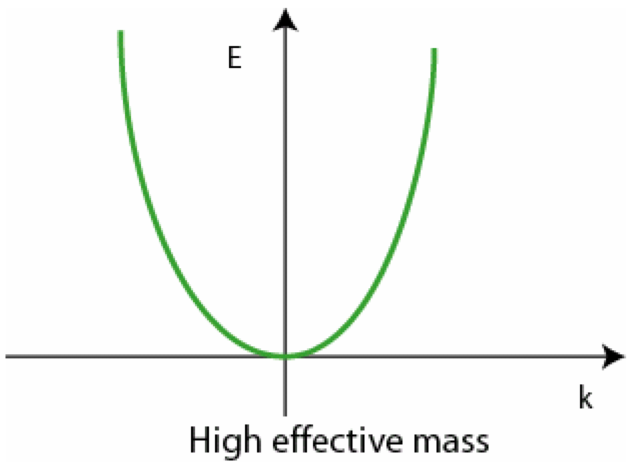
Electron in Free Space

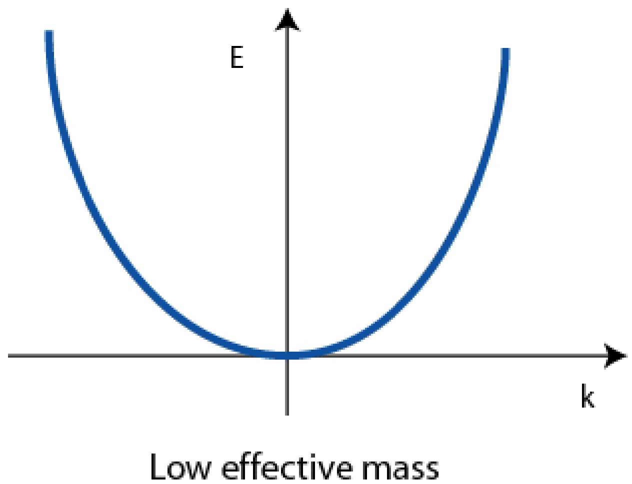
- Continuum of energy states – an electron can take on any energy
- Mass of the electron related to the curvature or second derivative of the energy-momentum diagram.

$$E = \frac{p^2}{2m}$$

$$\frac{d^2E}{dp^2} = \frac{1}{2m}$$

$$m_e^* = \left(\frac{d^2E}{dp^2}\right)^{-1}$$





Energy of Electrons

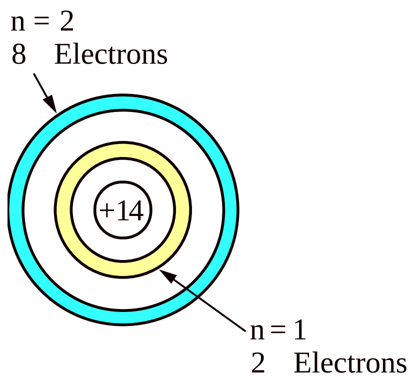
Atoms

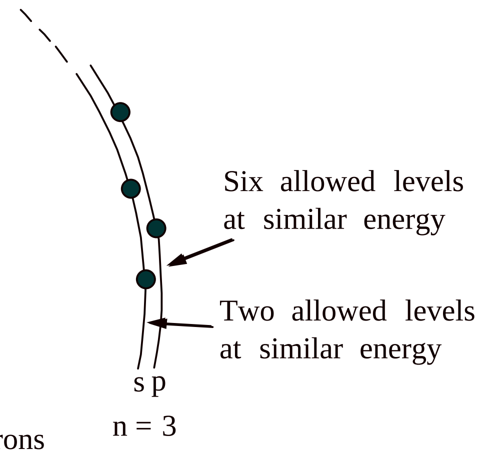
- Atom characterized by a coulombic attraction between the protons and the electrons

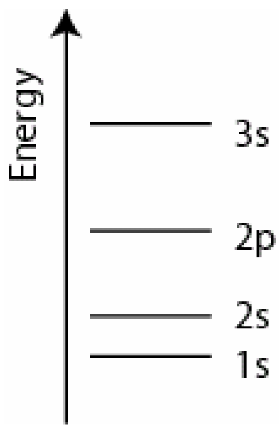
$$V = -\frac{q^2}{4\pi\varepsilon_0 r}$$

where q is the electronic charge and r is distance from the nucleolus.

- Solution to the Schrödinger Equation gives E as a set of discrete energy levels. These energy levels are characterized by the quantum numbers n, l, m, and s.



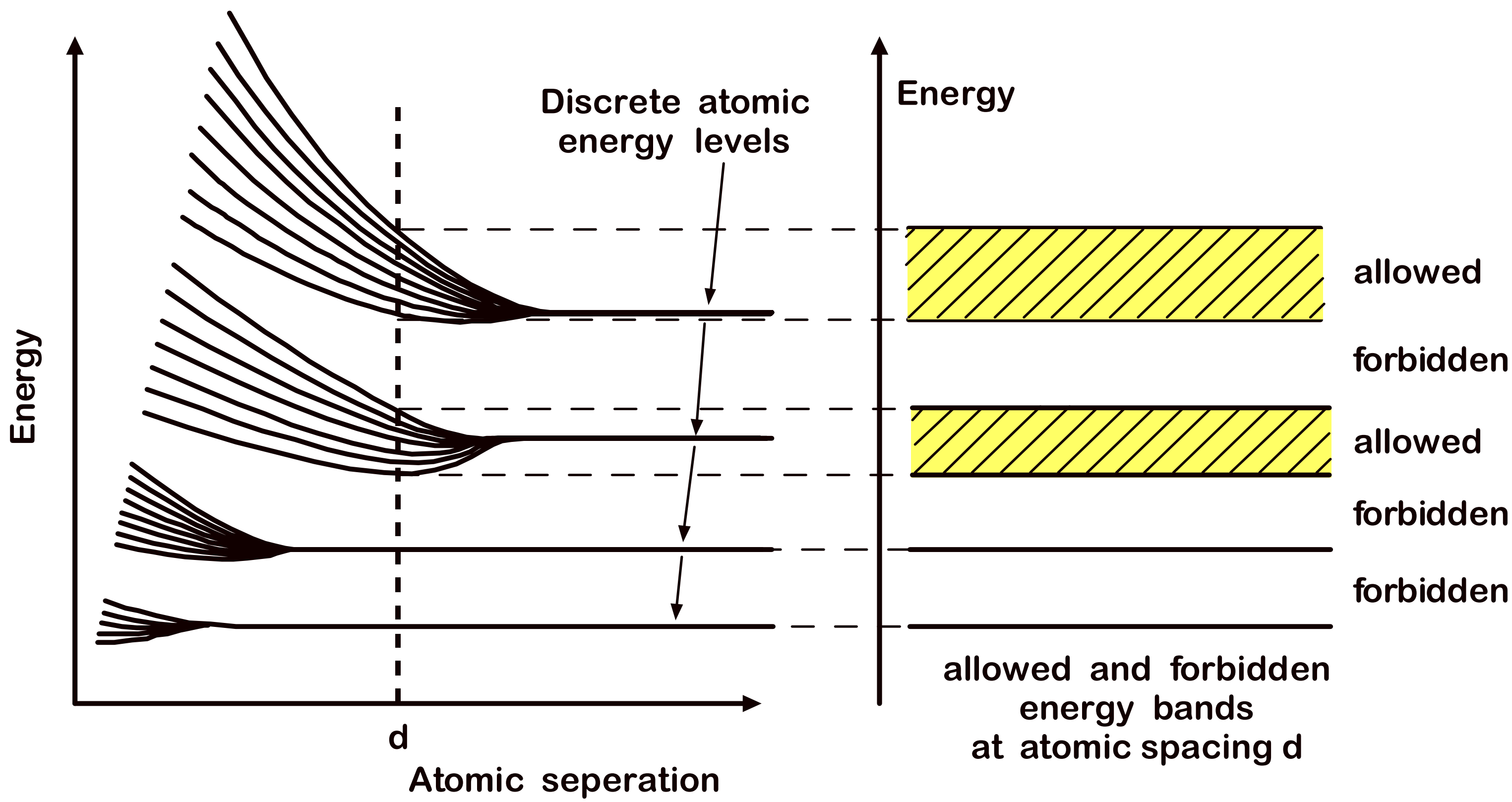




Band Diagrams

Formation of Energy Bands

- As more atoms interact, the splitting of the single energy levels forms bands of allowed and disallowed energy states.

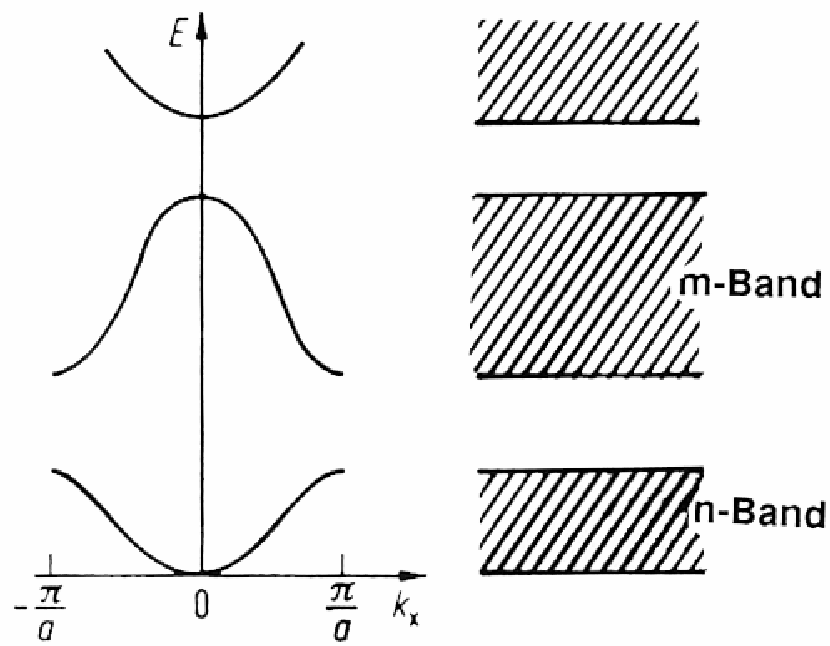


Dispersion Curves

Schrödinger Equation for Crystals

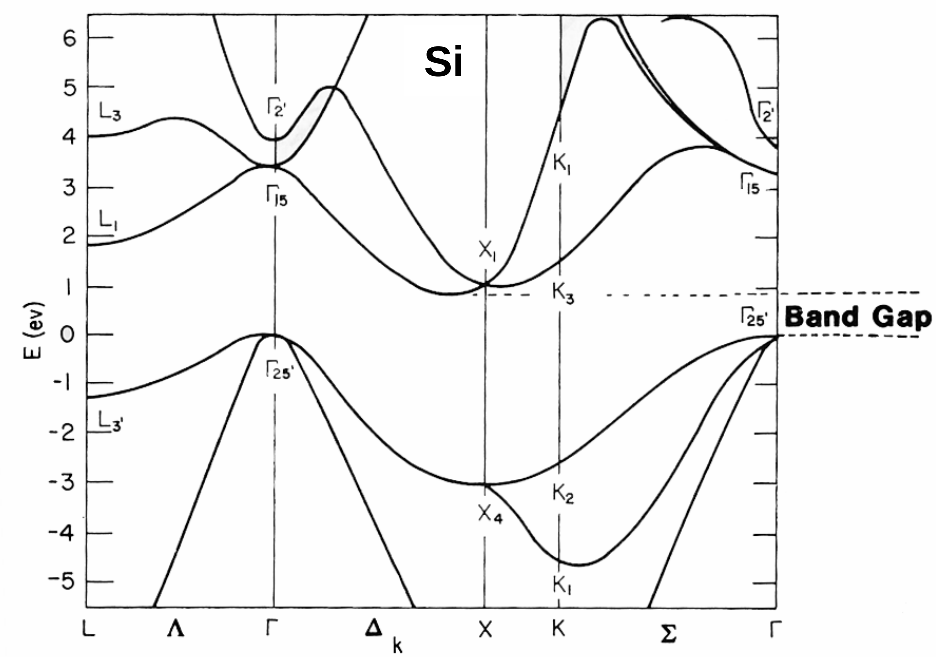
- Solution shows some energies have multiple energy states while some energies are disallowed.
- Electrons can only occupy places “on” the E-k diagram

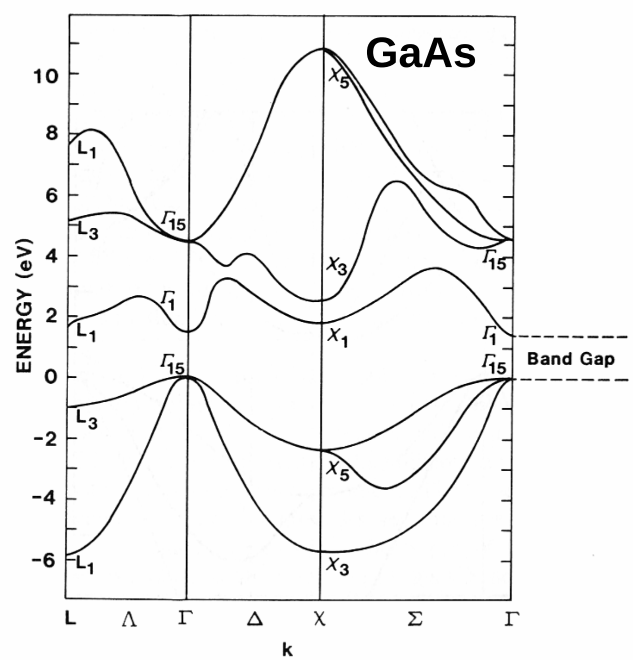
- The band gap is minimum difference between the two uppermost bands (conduction and valence band)
- Near the minima or maxima, bands are approximately parabolic, and hence can be approximated as “free” electrons
- Effective mass of each band near zone center varies, depending on its curvature
- Effective mass varies with k.



E-k diagrams

- In real crystals, the electrons move in three dimensions rather than one, and are described by three k-values rather than one.
- In E-k diagram, show band structure at a given point in the crystal lattice and has multiple energy bands.

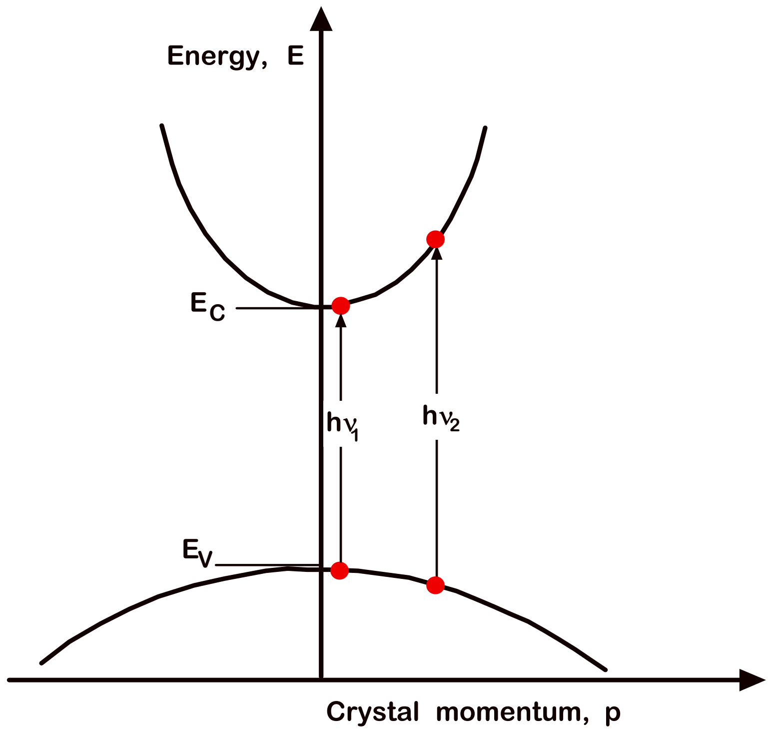




Direct and Indirect Band Gaps

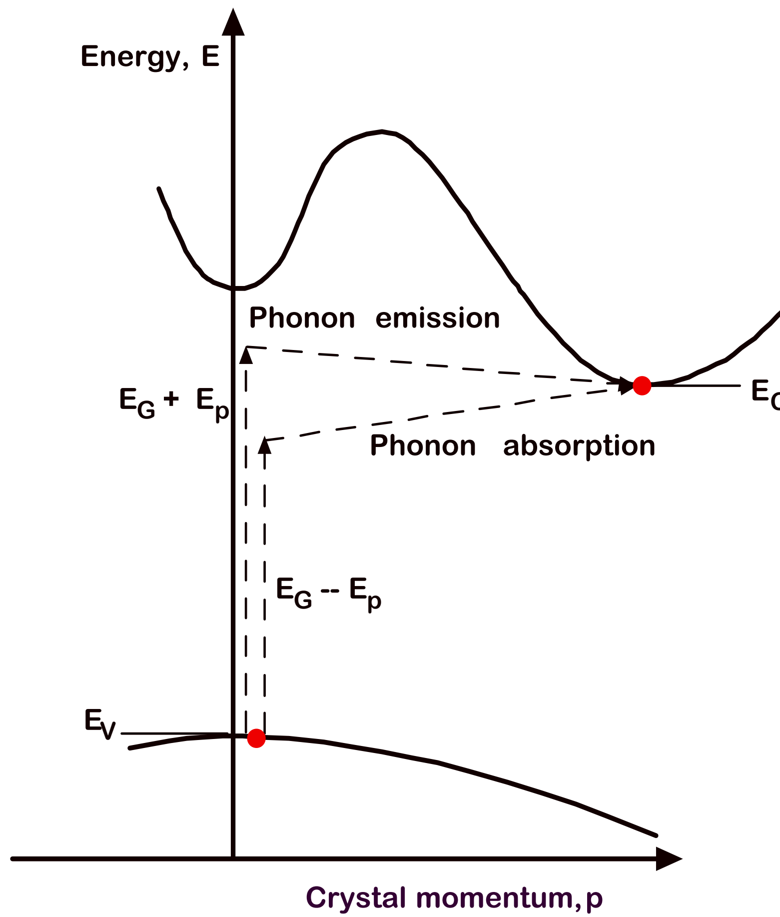
- The alignment of the conduction band minium and valence band maxima have a major impact on electrical properties such as absorption and recombination
- Aligned maxima and minima are called direct band gaps, misaligned are called indirect band gaps.

- **Direct Band Gaps**
  - The momentum at the energy CB minima is at the same as the VB energy maxima
  - To make a transition from the VB to the CB an electron requires a minimum energy E_G but its momentum remains unchanged
  - GaAs, InP and some other III-V semiconductors are examples of direct semiconductors .



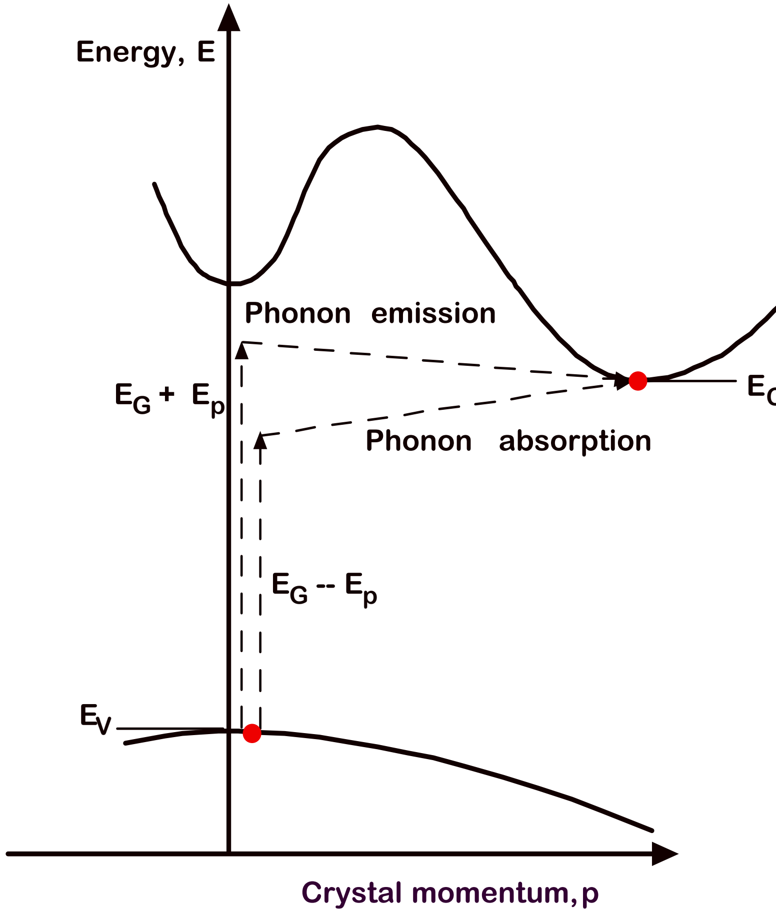
Direct and Indirect Band Gaps

- **Indirect Band Gaps**
  - **The CB minima does not correspond to the VB maxima**
  - **To make a transition from VB to CB an electron requires a minimum energy E_G plus a change in momentum.**
  - **Change in momentum requires interaction with a "heavy" particle, such as a phonon.**
  - **Examples of indirect band gaps are silicon (Si), germanium (Ge) and some III-V materials**



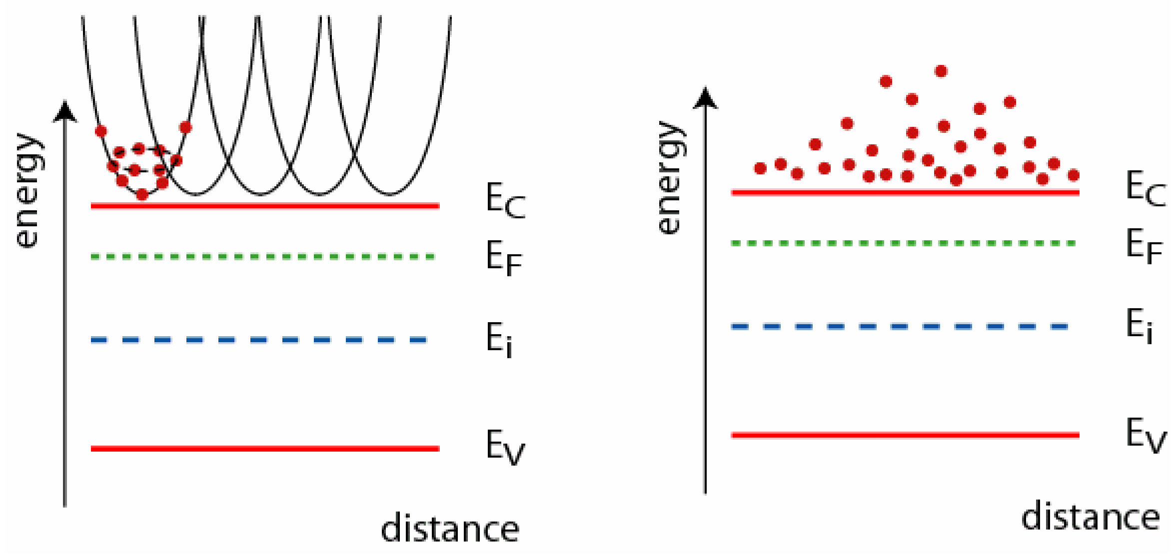
Summary of E-K Diagrams

- Information from E-k diagrams
  - Band gap: Energy between E_C minima and E_V maxima
  - Direct or indirect band gap: E_C minima and E_V maxima at same momentum
  - Effective mass: curvature of band
  - Density of states: change in energy/ change in number of quantum states.
  - Absorption coefficient
  - Mobility: shape and curvature of bands



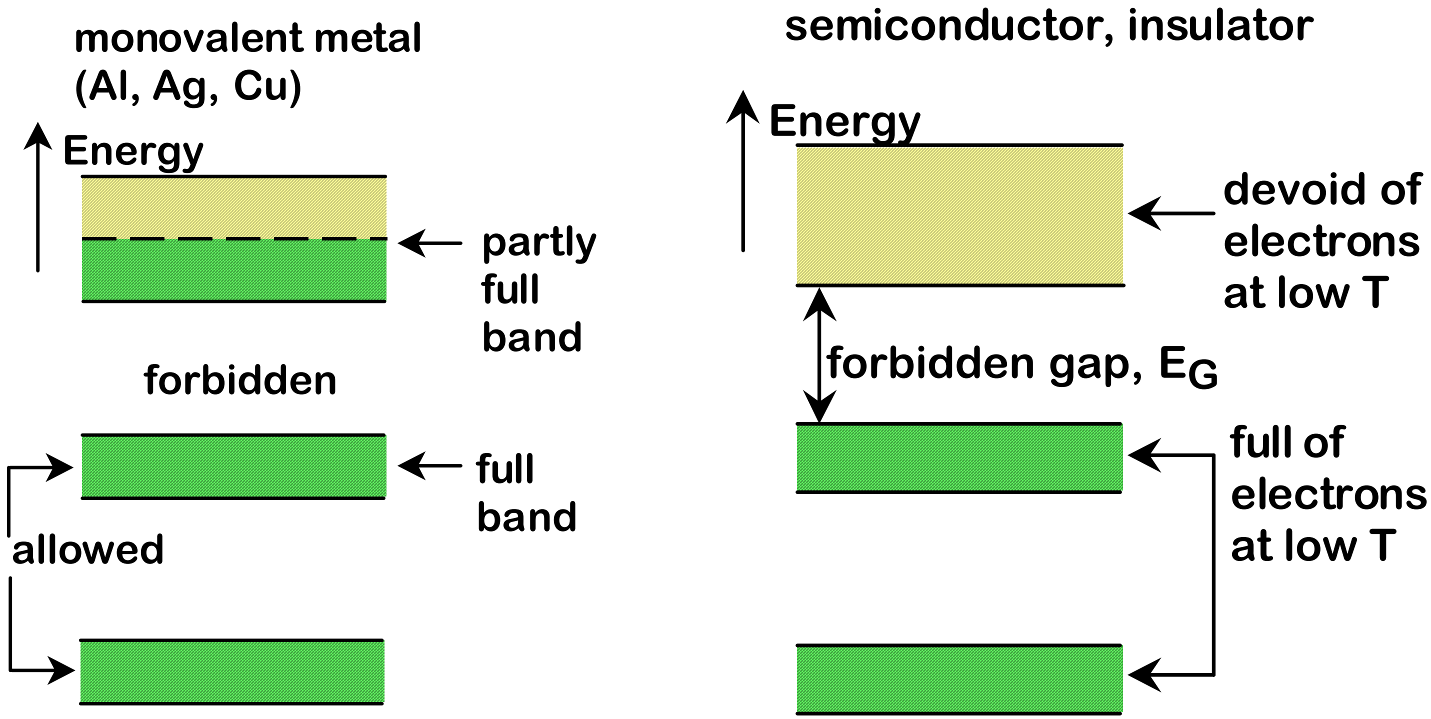
Reduced Energy Bands

- **In many cases in semiconductor devices, we do not need to take into account change in momentum or exact distribution of carriers with energy.**
  - **For example, if carriers are not significantly disturbed from the VB maxima or CB band minima, then they act like free electrons.**
  - **Density of States gives the number of electron states as a function of energy**



Metals and Semiconductors

- The difference between a metal, insulator and semiconductor is the band gap and number of electrons in the outer most band.
- For a metal, the bands can either overlap or be partially filled, so the number of carriers for conduction is high

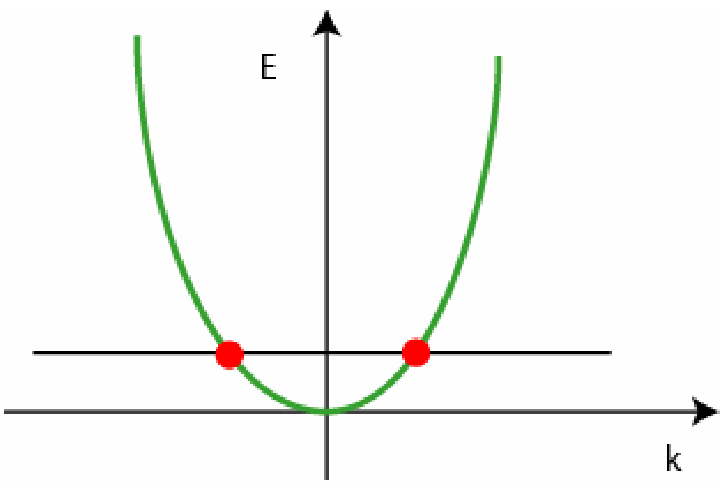


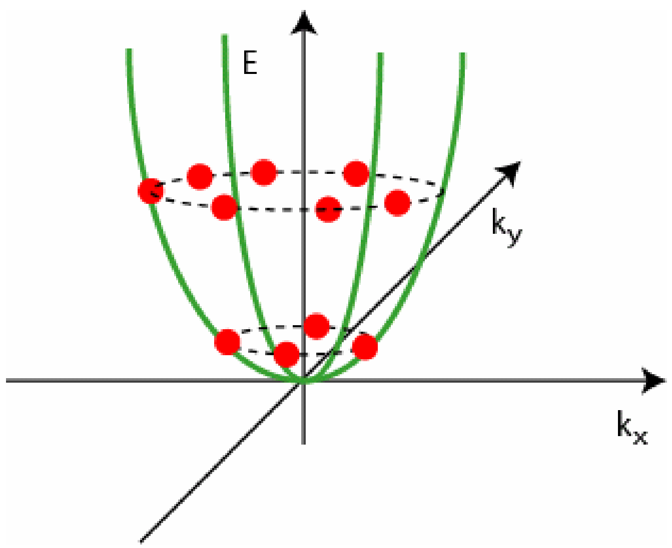
Carrier Concentrations

- Once we have found the allowed energy states for electrons in a semiconductor, we need to find the number of carriers that are in the crystal.
- Find the total number of carriers by:
  - Finding the maximum number of possible carriers that are allowed at each particular energy – this function is called the density of states
  - Find the probability that there is a carrier occupying a particular energy level – this is given by the Fermi function.

Density of States

- The density of states depends on the number of allowed electrons per energy per volume.
- Looking for total number of energy states, regardless of the momentum of the electrons.
- We need to find two relationships: between E and k (from the E-k diagram) and the number of k states per volume.



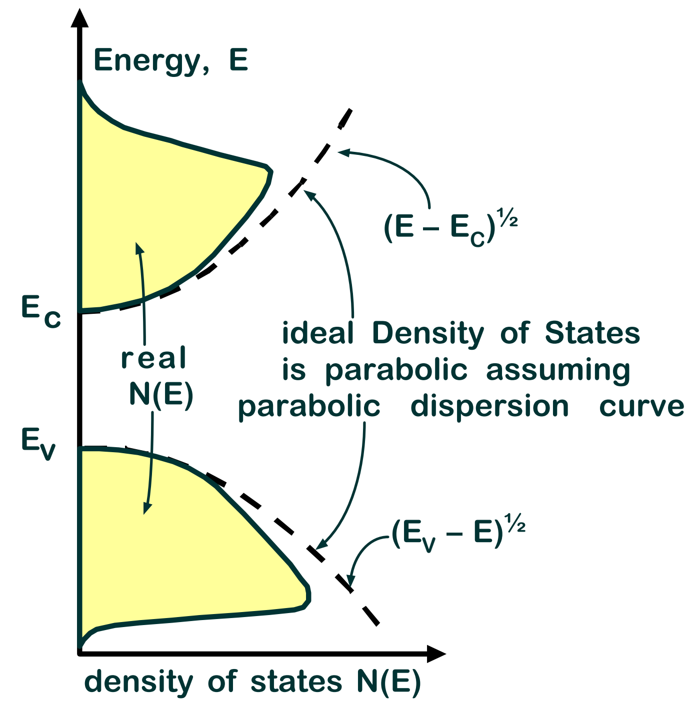


Density of States

- The density of states gives the maximum number of electrons that can occupy a given band, not necessarily the number that do exist.
- Density of States N(E) for real bands goes to zero at higher energies due to non-parabolic nature of bands
- Smaller N(E) at lower energy affects absorption and emission for opt-electronic devices.

$$N_C(E) = \frac{4\pi\left(2m_n^*\right)^{3/2}}{h^3}\sqrt{E - E_C}$$

$$N_v(E) = \frac{4\pi\left(2m_p^*\right)^{3/2}}{h^3}\sqrt{E_V - E}$$

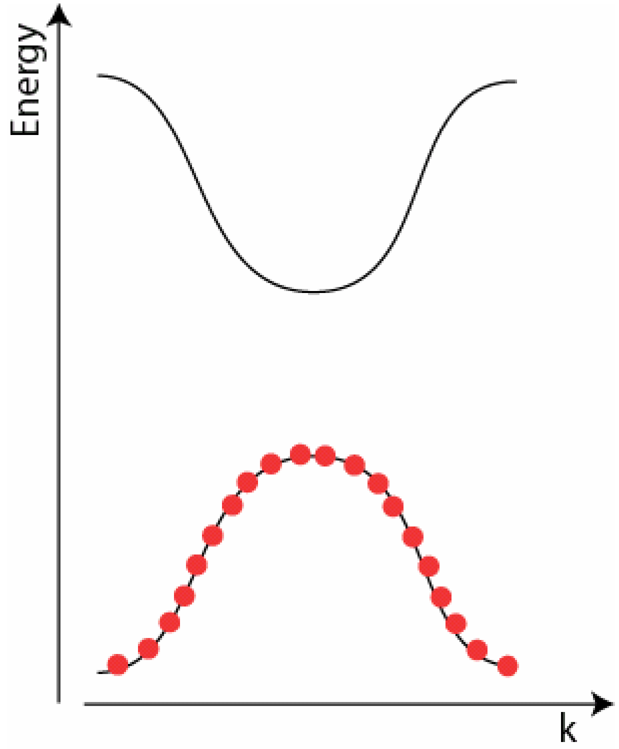


Electron Population in Bands

- Central to the properties of electrons are that they are in constant, random motion and in thermal equilibrium with other electrons and lattice.
  - At absolute zero, the extra energy of the carriers is zero, and all the electrons occupy their lowest energy position.
  - The temperature of a collection of electrons is given by an average energy (temperature) – we cannot know the energy of each electron, but its total average energy remains the same.
  - Because of their temperature, some electrons will occupy higher energy states in the band diagram, leaving empty states at lower energy. The electrons only stay at the higher energy for a short time, eventually going back down to their lower energy position.
  - The electrons give off their energy to another electron, which can then occupy a higher energy state.

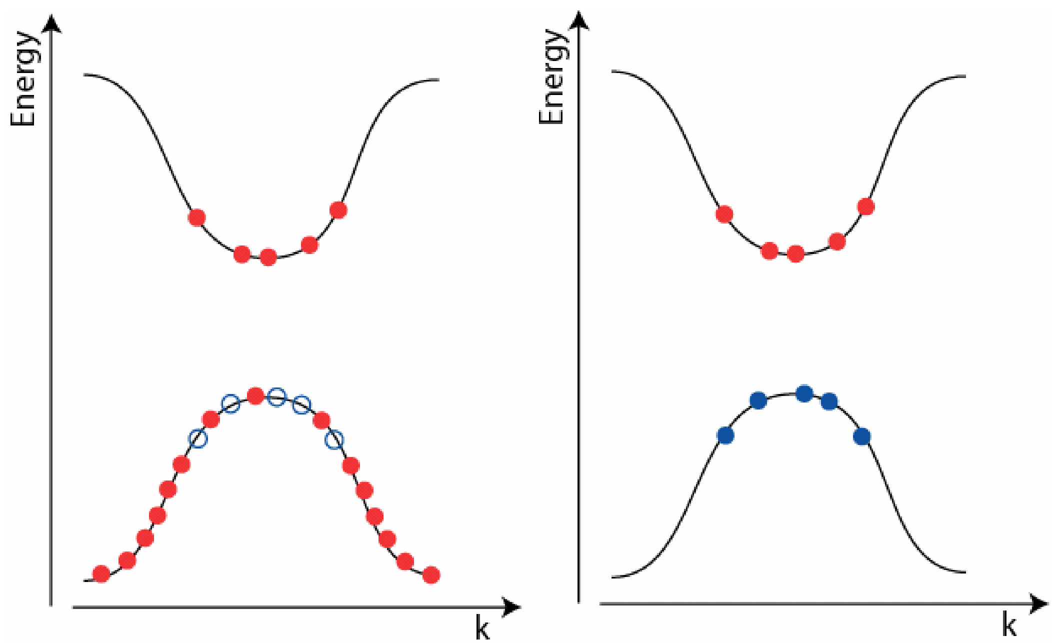
Free Electrons

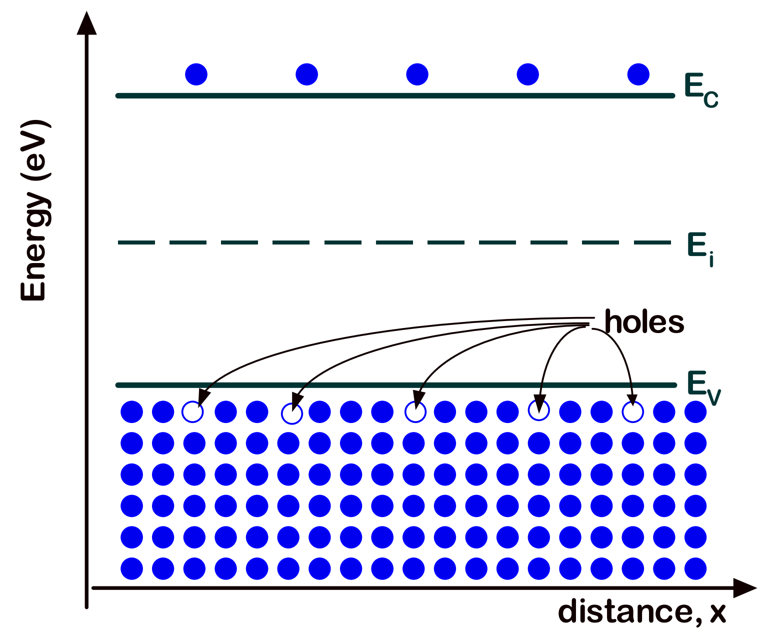
- Since we are interested in current flow or how electrons change their energy, we are ONLY interested in the number of electrons that can participate in conduction or change their energy.
- In order to have a current flow, electrons must be able to move to another spot and gain energy.
- Electrons in a completely full band cannot participate in conduction.
  - For semiconductor and insulators, at 0K, the uppermost band (valence band) is completely full of electrons.
  - Electrons in the next uppermost band (conduction band) can participate in conduction.
  - No free electrons when band is full



Free Electrons and Holes

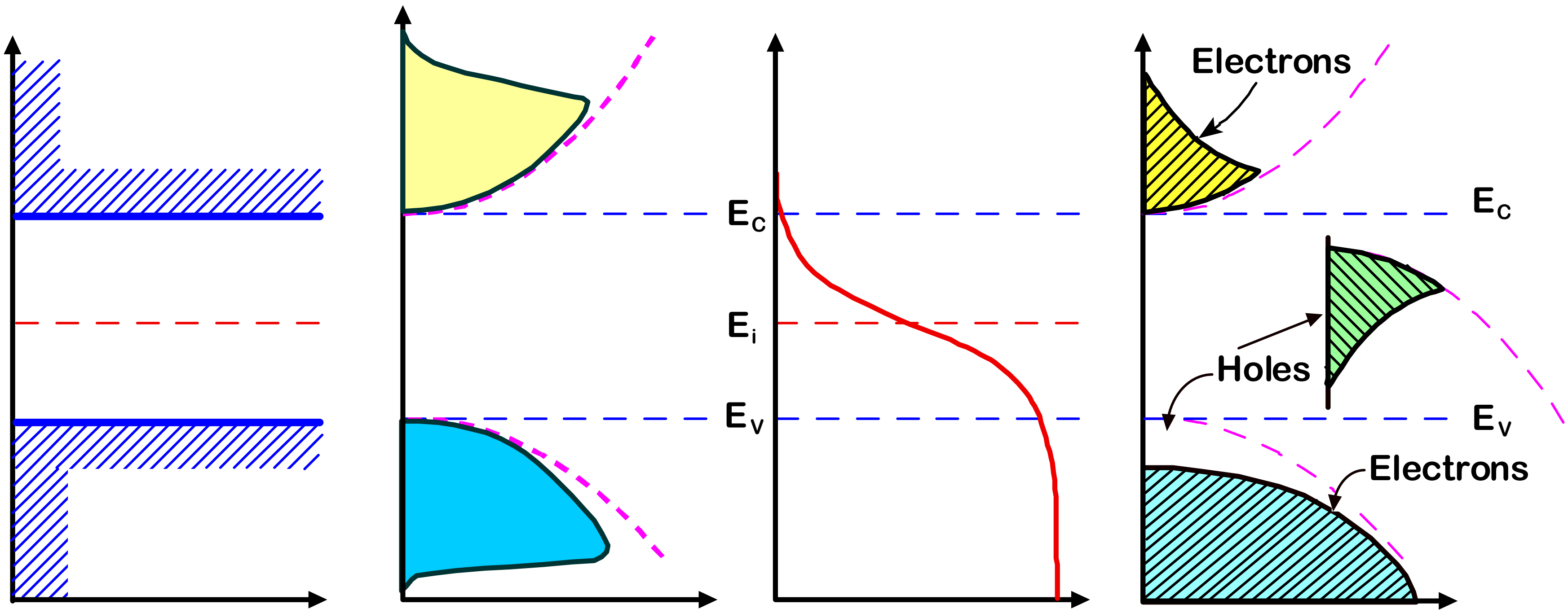
- When electrons move to the CB, they leave behind empty states and other electrons in the VB can move into these empty states.
- The total number of electrons that can move is the number in CB and number of empty states in VB, and empty states called holes.
- Holes have different masses, motilities.





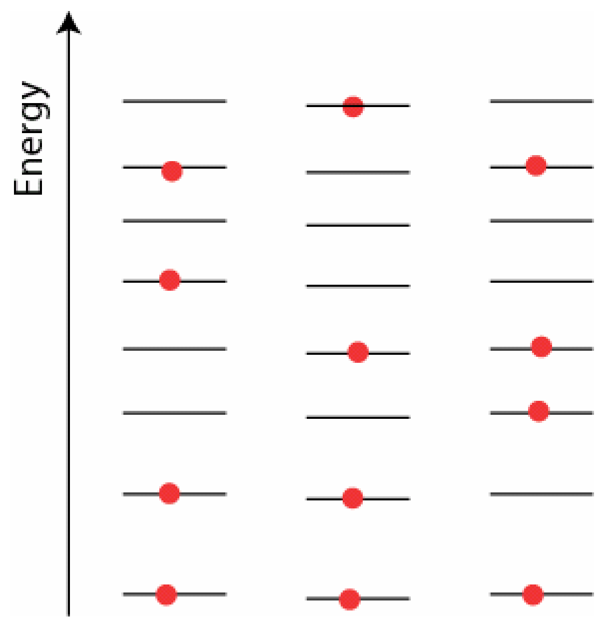
Number of Carriers

- Can find the number of carriers by multiplying the maximum number of carriers at each energy by the probability of having that state occupied and integrating.



Fermi Distribution

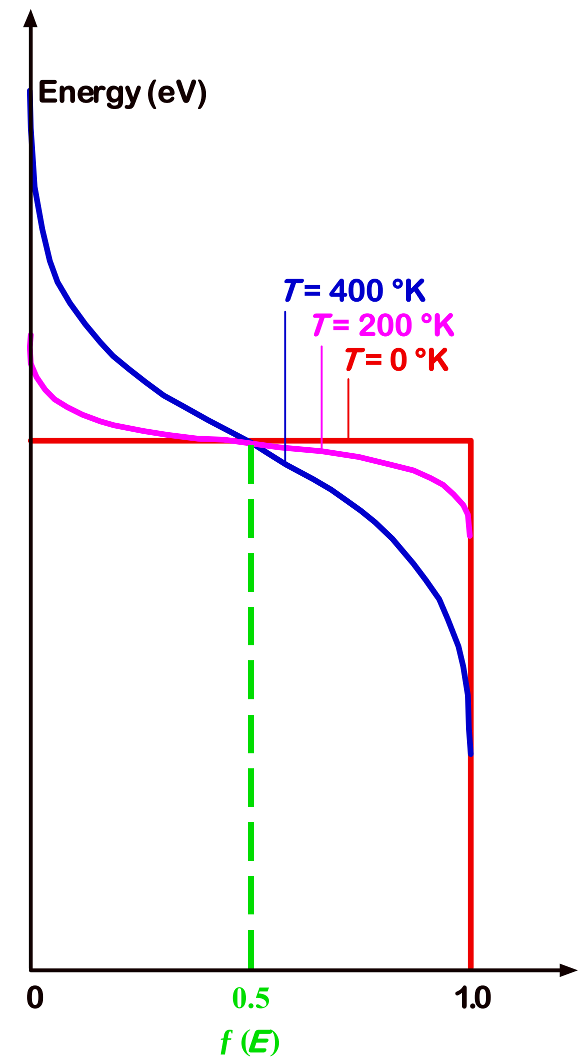
- The final piece of information we need to calculate the number of free electrons is the probability distribution function as a function of energy – I.e, how likely they are to occupy each energy level.
- To determine the probability function, we determine the total number of ways that N electrons can fill a given number of energy states, while keeping their total energy constant.
- In most cases, the lowest energy levels are filled – they have a high probability of being occupied.
- Higher energy states less likely to be filled
- Math involves determining total number of ways that can put N electrons into a a given number of energy states at a fixed total energy



Fermi Distribution

- The resulting probability distribution function is called the Fermi-Dirac distribution function:

$$f(E) = \frac{1}{1 + \exp\left({(E - E_F)}/{kT} \right)}$$



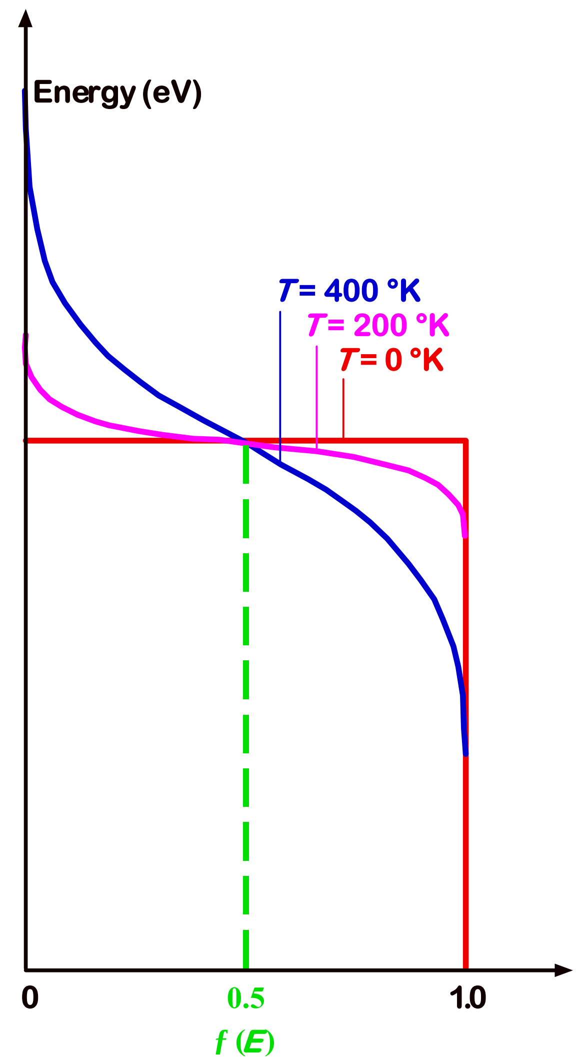
- The Fermi-Function is the probability that an electron will occupy a given energy state E.
- The Fermi-function is symmetric since if a higher state is occupied, a lower state must necessarily be unoccupied
- It depends *only* on the number of carriers and the thermal energy of the system - it does not take into account that a given energy state may be allowed or disallowed.

Fermi Function

- The Fermi function depends on temperature, since at higher temperatures, the probability of a higher energy state being occupied is higher.

$$f(E) = \frac{1}{1 + \exp\left(\left(E - E_F\right)/kT\right)}$$

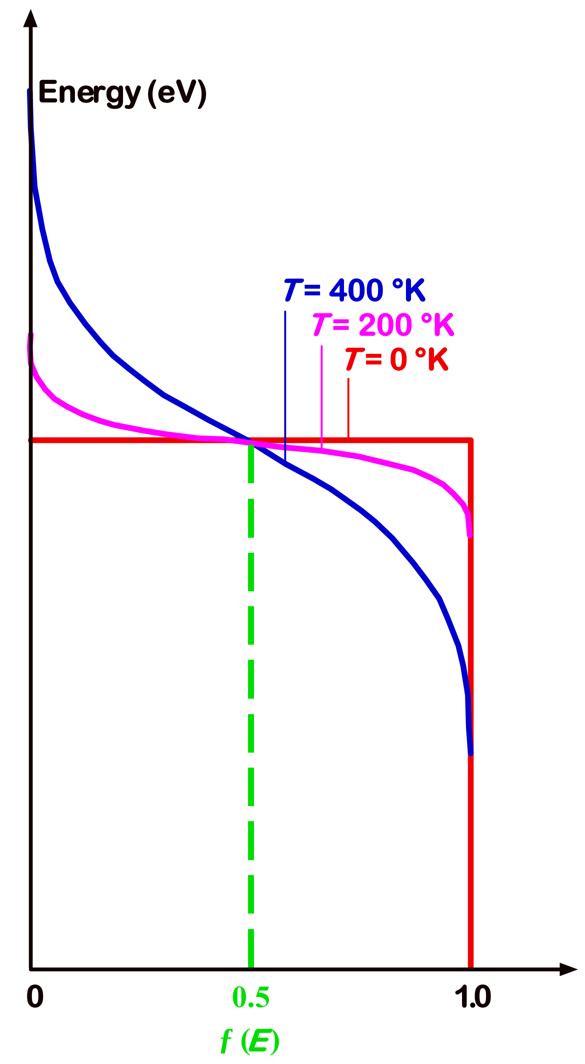
- At 0K, the probability distribution is square since we can predict exactly the energy position of each electron.



Fermi Level

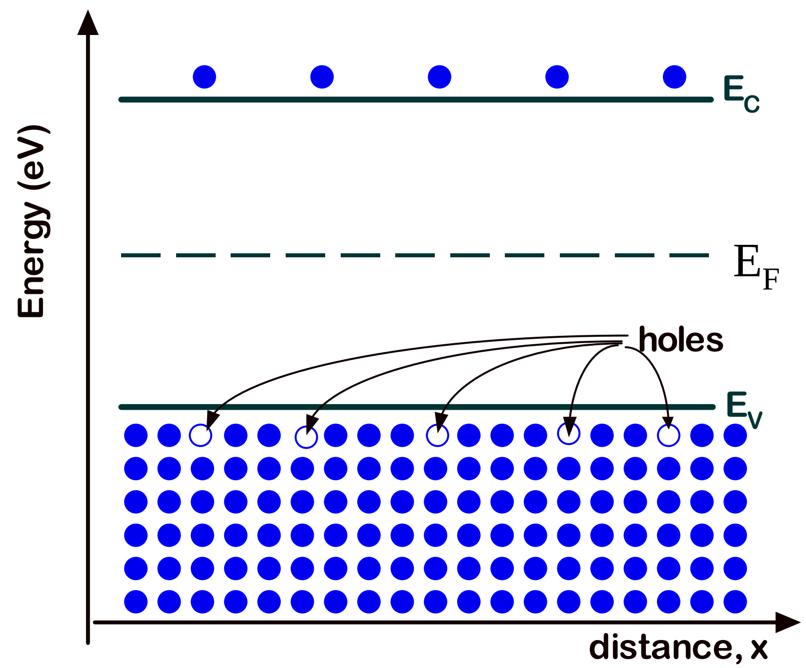
- The Fermi-function depends on the temperature and the number of electrons in the system, and the Fermi-level, E_F, is related to the number of electrons in the system.
- Assuming that the number of electrons stays constant with temperature, then E_F does not change with temperature.
- Mathematically, E_F is defined as the energy at which the probability of occupation is ½.

$$f(E = E_F) = \frac{1}{1 + \exp\left({(E - E_F)}/{kT} \right)} = 0.5$$



Fermi Level

- Fermi-level for holes is $f_h(E) = 1 - f(E)$, since probability of a hole occupying an energy level is 1 – probability of an electron occupying that energy level.
- Fermi-level has several physical interpretations.
  - Average energy of the FREE carriers in the system.
    - In equilibrium, the average energy just always be the same, so E_F must be constant.
  - Filling level of electrons in the system, and hence number of electrons (and holes)in the system.



Approximations to Fermi function

- Fermi function can be difficult to use in anything but numerical calculations.

$$f(E)=\frac{1}{1+\exp\left(\left(E-E_F\right)/kT\right)}$$

- In analysis, usually approximate the Fermi-function as:

$$f(E)=\frac{1}{1+\exp\left(\left(E-E_F\right)/kT\right)}\approx\frac{1}{\exp\left(\left(E-E_F\right)/kT\right)} \qquad \frac{(E-E_F)}{kT}>3 \quad \text{or } (E-E_F)>3kT$$

- Called Maxwell-Boltzman approximation
- A degenerate semi-conductor is one which has

$$(E_C-E_F)<3kT$$ N-type

$$(E_F-E_V)<3kT$$ P-type

Number of Carriers

- **Mathematically:**

$$n = \int_{E_C}^{E_{MAX}} N(E) f(E) dE$$

$$N_C(E) = \frac{4\pi\left(2m_n^*\right)^{3/2}}{h^3}\sqrt{E - E_C} \qquad f(E) = \frac{1}{\exp\left(\left(E - E_F\right)/kT\right)}$$

$$n = N_C \exp\left[\left(E_F - E_C\right)/kT\right]$$

where

$$N_C = 2\left(\frac{2\pi m_e^* kT}{h^2}\right)^{3/2} M_C$$

- **Similarly for holes in the valence band:**

$$p = N_V \exp\left[\left(E_V - E_F\right)/kT\right]$$

where

$$N_V = 2\left(\frac{2\pi m_h^* kT}{h^2}\right)^{3/2} M_V$$

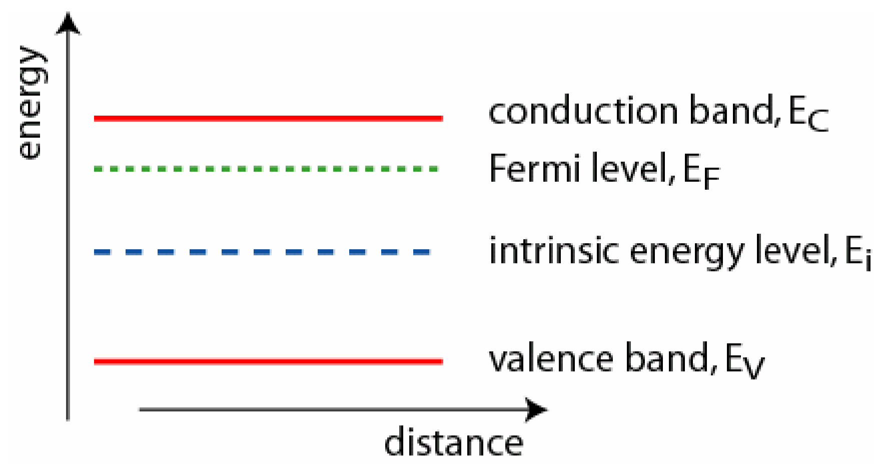
Intrinsic Energy Level

- The Fermi-level for an intrinsic semiconductor called intrinsic energy level or E_i
- An calculate E_i by noting that for an intrinsic semiconductor, $n=p=n_i$
- Ei is a better reference energy than EC or EV in cases where there are multiple band gaps or where there the are regions where the number of electrons and holes both need to be calculated.

$$n = p = n_i$$

$$N_C \exp\left[{(E_i - E_C)}/{kT}\right] = N_V \exp\left[{(E_V - E_i)}/{kT}\right]$$

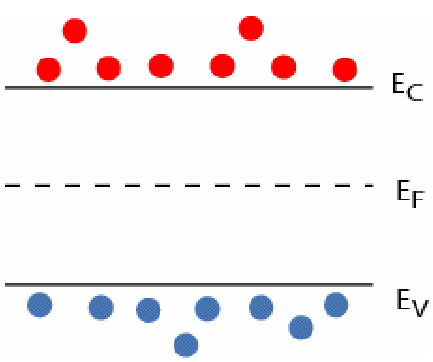
$$E_i = \frac{(E_C + E_V)}{2} + \frac{kT}{2} \ln\left({N_V}/{N_C}\right)$$

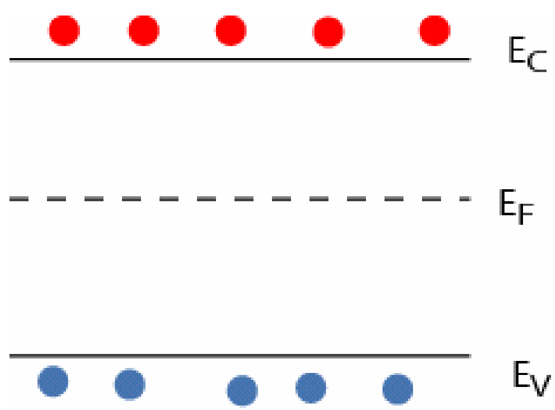


Law of Mass Action

- Without doping, the electron and hole concentration must be equal in equilibrium. This carrier is called intrinsic carrier concentration, n_i.
- n_i depends on E_G, temperature and effective mass.
- Law of Mass Action relates n and p to n_i.
  - Holds for any doping, but ONLY in equilibrium

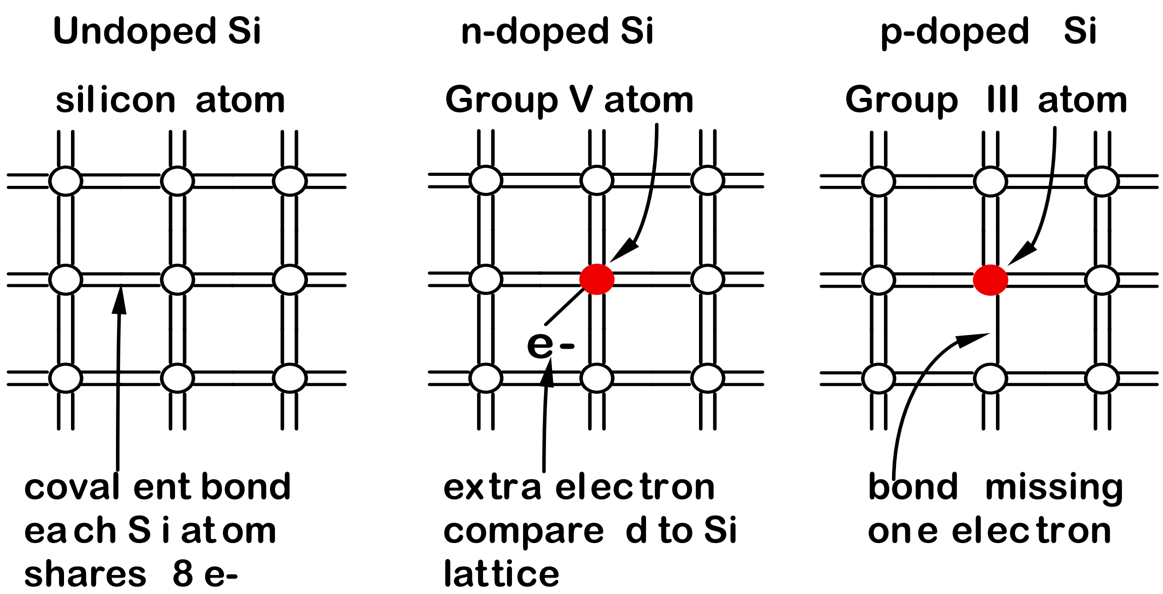
$$np = N_C \exp\left[{(E_F - E_C)}/{kT}\right] N_V \exp\left[{(E_V - E_F)}/{kT}\right] = n_i^2$$





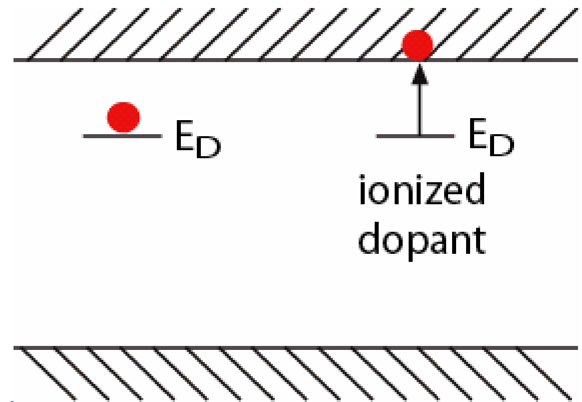
Doping

- Semiconductors are unique in that the carrier concentrations can be altered by doping.
- Can change the number of electrons or holes by adding materials to the silicon lattice that have extra or less electrons.
- A doped semiconductor is electrically neutral, but the number of free electron or hole concentrations change.
- N-type (n for negative doping has extra electrons
- P-type (p for positive has extra holes
- Need to determine modified carrier concentrations

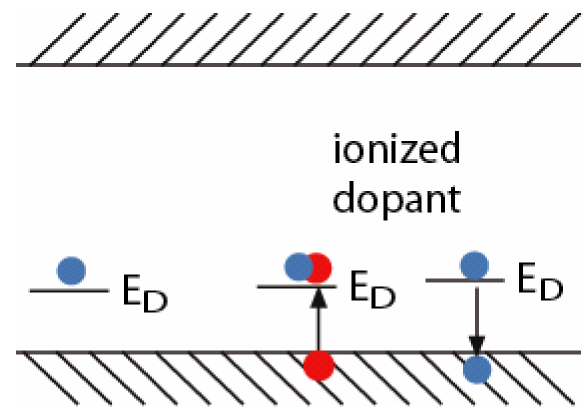


Doping

- Doping introduces allowed energy states into the forbidden region in the band gap.
- The electron can move from its energy level (E_D) to E_C if:
  - The electron has enough thermal energy
  - There is an empty space in the conduction band.

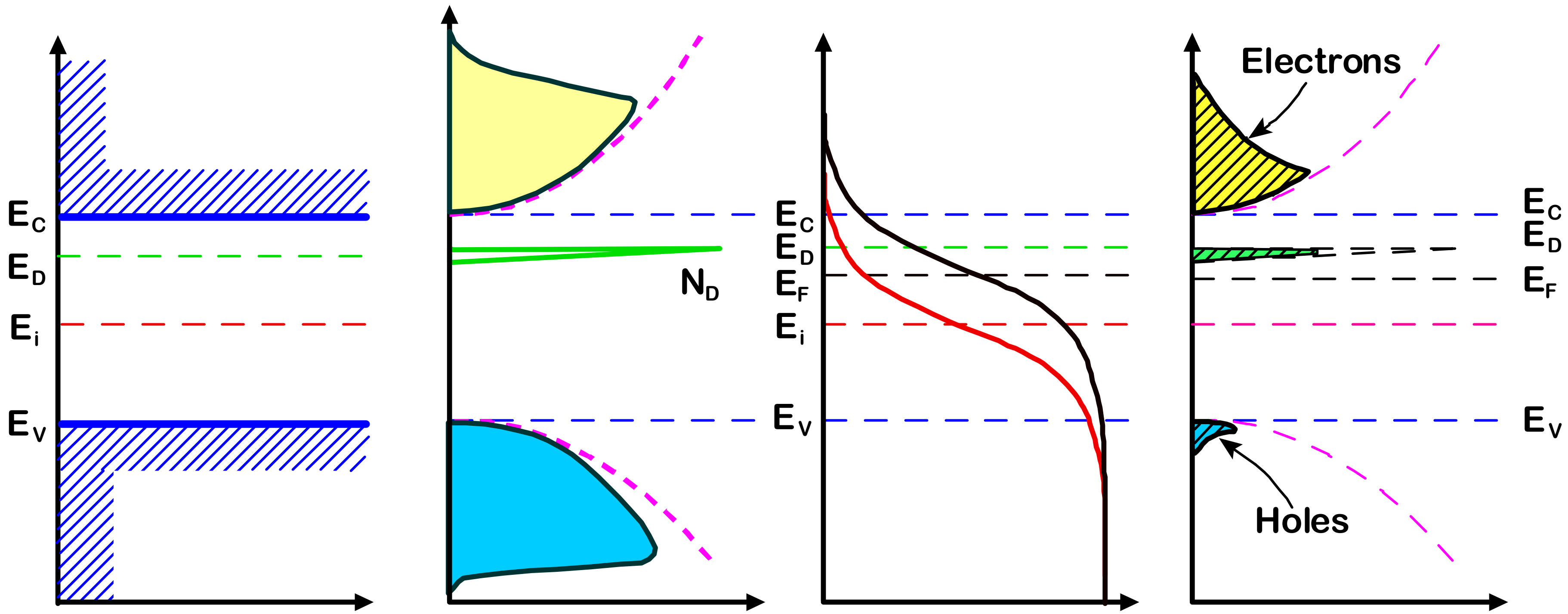


- A dopant atoms that has released its electron to the conduction band is called ionized.
- Similar process with p-type doping, expect that an electron from valence band moves into the empty space, leaving behind a hole in the valence band



Doping

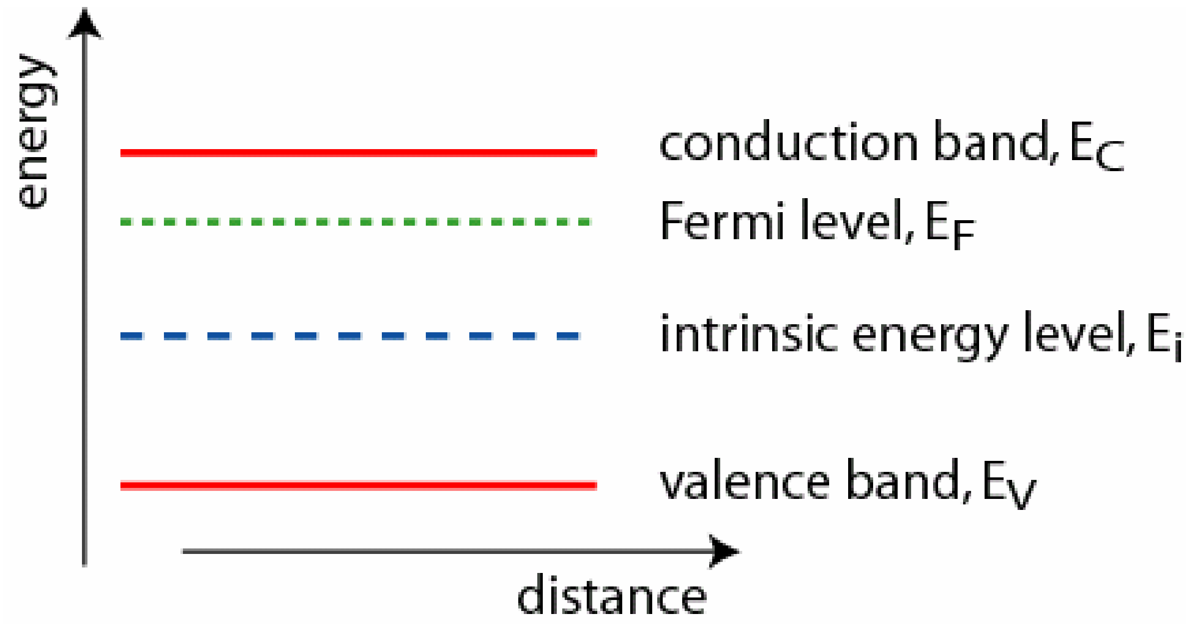
- Determine total number of carriers same way as intrinsic case



- Fermi-level increases, number of electrons increase and number of holes decreases.

Energy Band Diagrams

- Should previously have seen and used simple band diagram.

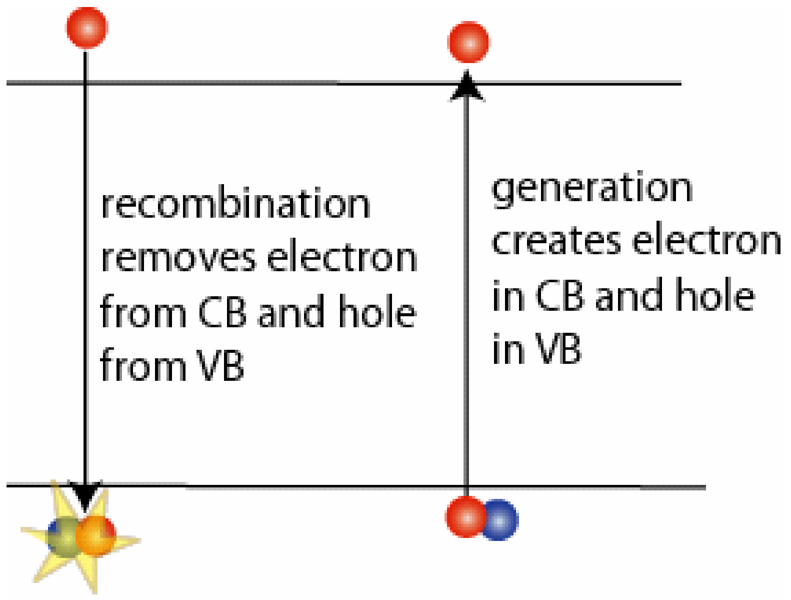


Recombination & Generation

- **Outline:**
  - Carrier concentrations are altered from a piece of bulk material in equilibrium by two factors:
    - Generation and recombination of carriers
    - Transport of carriers from one region to another.
  - Need to determine processes for recombination and generation, and their rates.
  - Need to determine the processes for transport, and how they depend on the carrier concentrations.
    - We will consider drift and diffusion as the transport processes.

Generation & Recombination

- Even with no external inputs, carriers are continuously moving from band to band, but at equilibrium, the carrier concentration does not change as a result of these processes.
- Generation refers to any process by which electrons move from valence band to conduction band to conduction band, leaving behind a hole in valence band.
- Recombination is any process by which electrons from conduction band move back into the valence band, thereby removing a hole from the valence band.



Generation: Basic Processes

- In order to move from one band to another, there are several requirements:
  - Carrier must gain enough energy to move from one band to another
  - There must be an electron in the valence band or at another low energy level.
  - There must be an unoccupied space to which the electron can move.
- Energy can come from thermal energy or from photons.
  - Unless there is a thermal gradient across the material, thermal energy does not cause a net generation rate, as it is balanced by recombination.
  - Hence, will only consider generation due to photons.
- Every recombination process has an inverse generation process, but not all are practically observed.

Generation: Photons

- Photons are quantum mechanical particle that describes electromagnetic radiation.
- Properties of photons:
  - Photons have small momentum, but large energies.
  - Energy given by either energy (usually in eV) or by wavelength or frequency.

$$E = \frac{hc}{\lambda} = h\nu$$

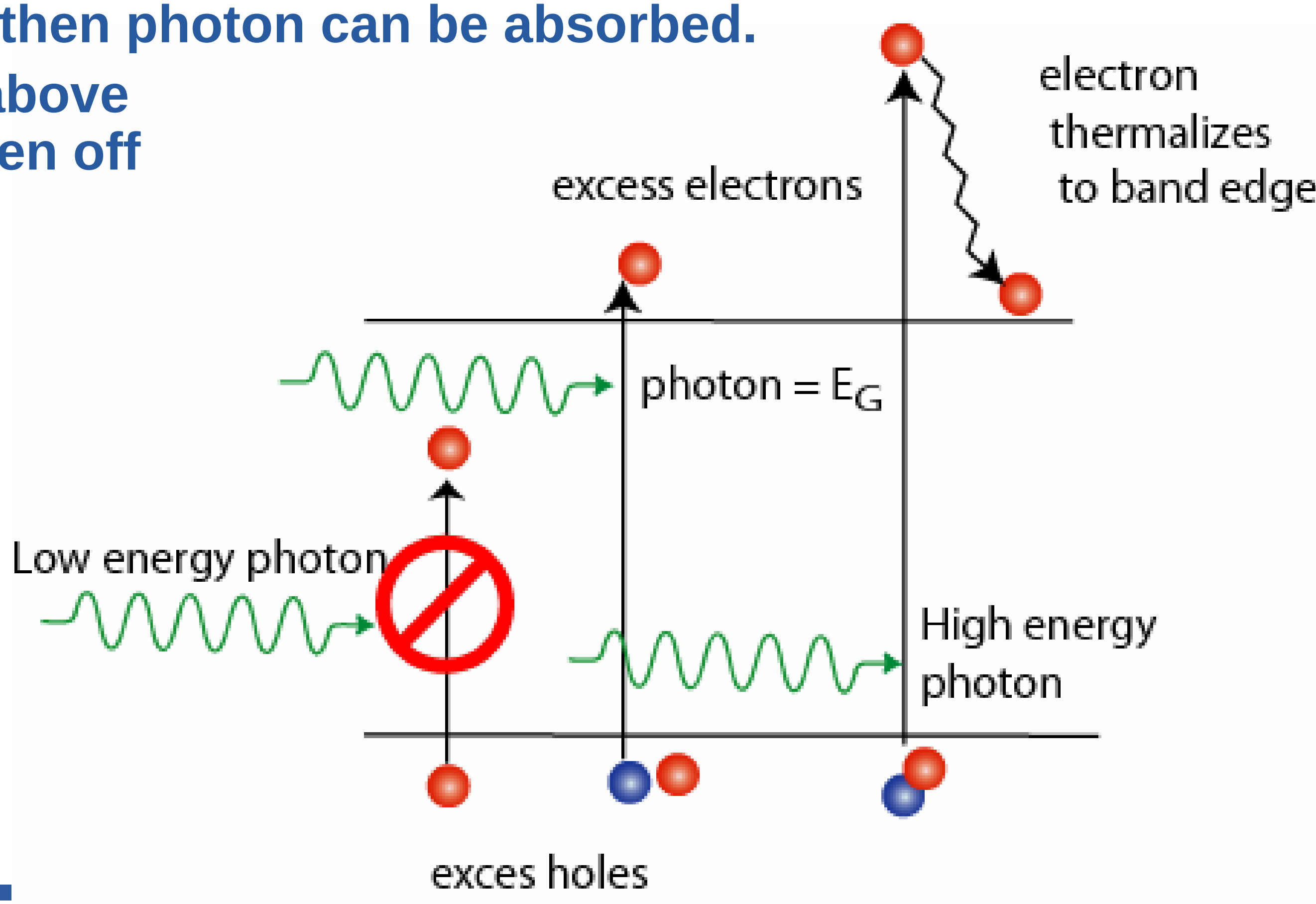
  - Photon flux gives number of photons/sec.cm²
  - Can convert between photon flux and power density (for a monochromatic source) by:

$$H\left(\frac{W}{m^2}\right) = \frac{\#\ photons}{sec\ m^2} \times \frac{E(J)}{photon} = \Phi E(J) = \Phi\frac{hc}{\lambda}$$

$$H\left(\frac{W}{m^2}\right) = \Phi E(J) = q\Phi E(eV) = q\Phi\frac{1.24}{\lambda}$$

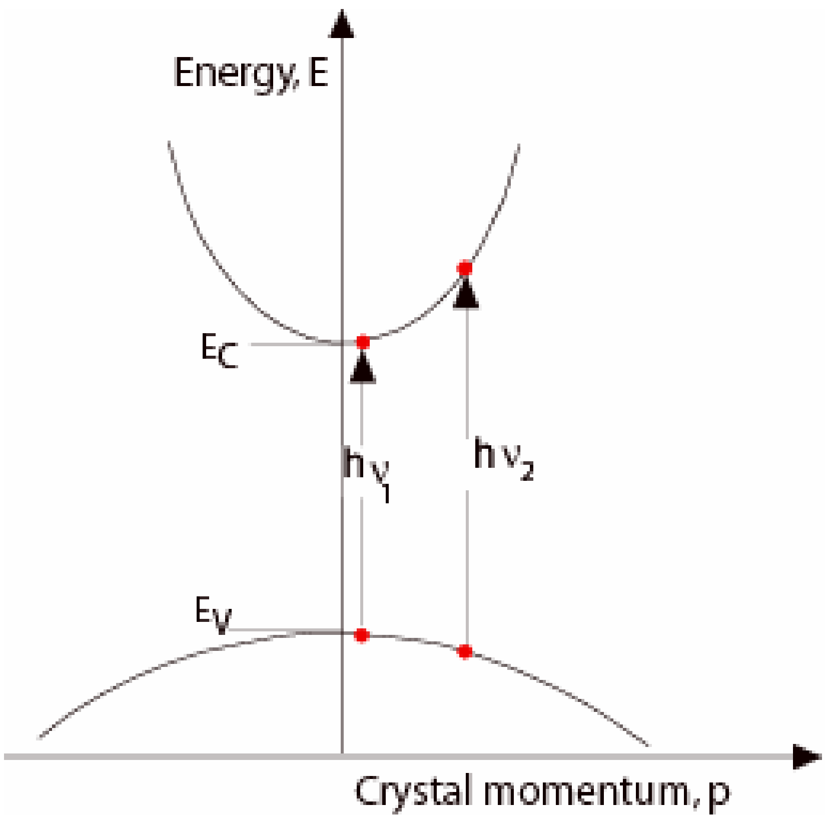
Generation: Photons

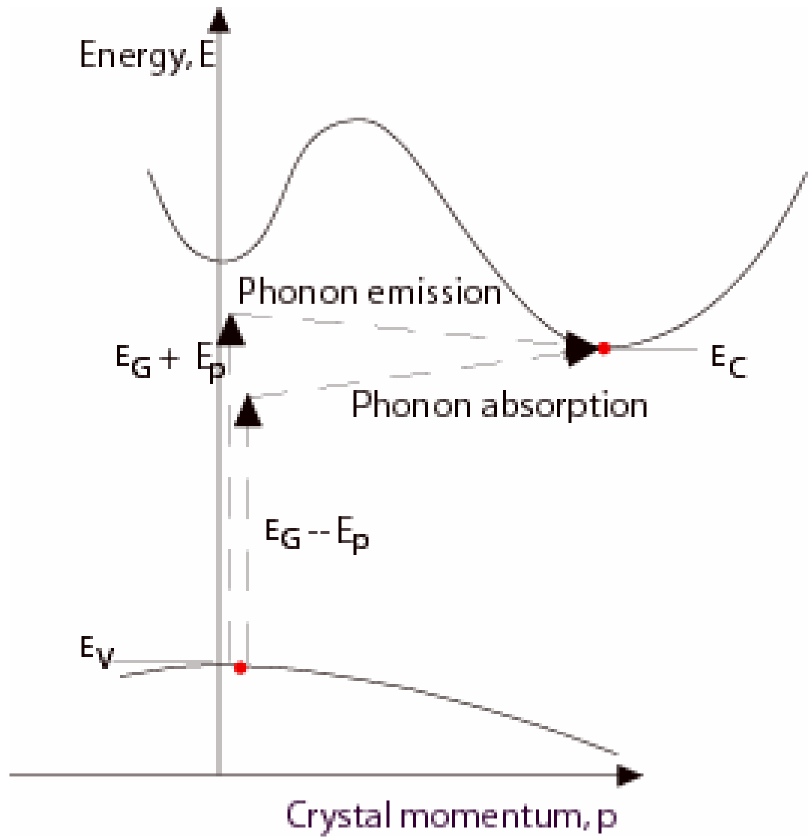
- **The energy of a photons has a major impact on how the photon interacts with the semiconductor.**
- **If the photon <E_G, then ideally no generation**
- **If photon >= E_G, then photon can be absorbed.**
- **Excess energy above Eg generally given off as heat**



Generation: Band to Band

- **Band-to-band generation can occur via either direct or indirect transitions.**



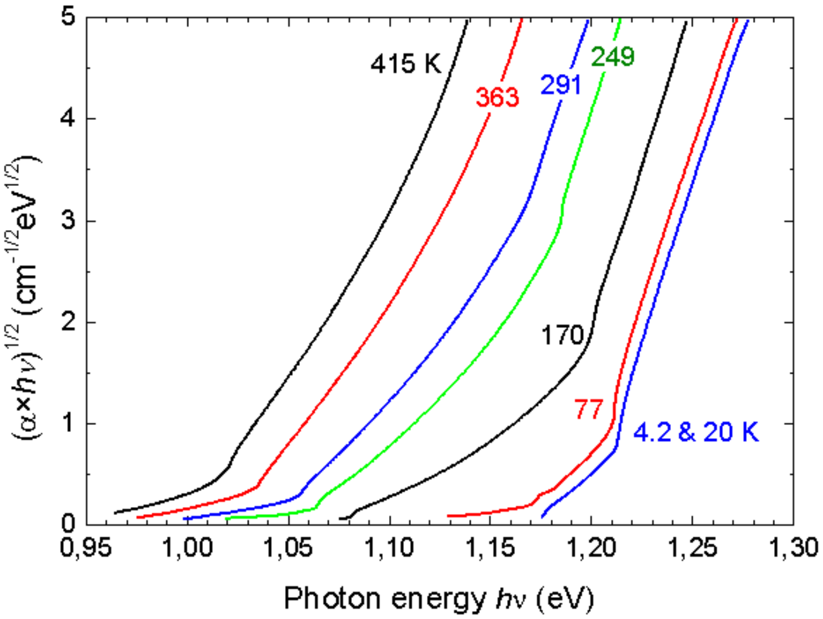


Generation: Absorption coefficient

- **Absorption coefficient, α, is a measure of the probability of absorbing a given photon.**
- **Absorption depends on the likelihood of the transition occurring – lower for processes near the band edge, increasing for higher photon energies.**
- **For band-to-band transitions, the absorption coefficient has the form**

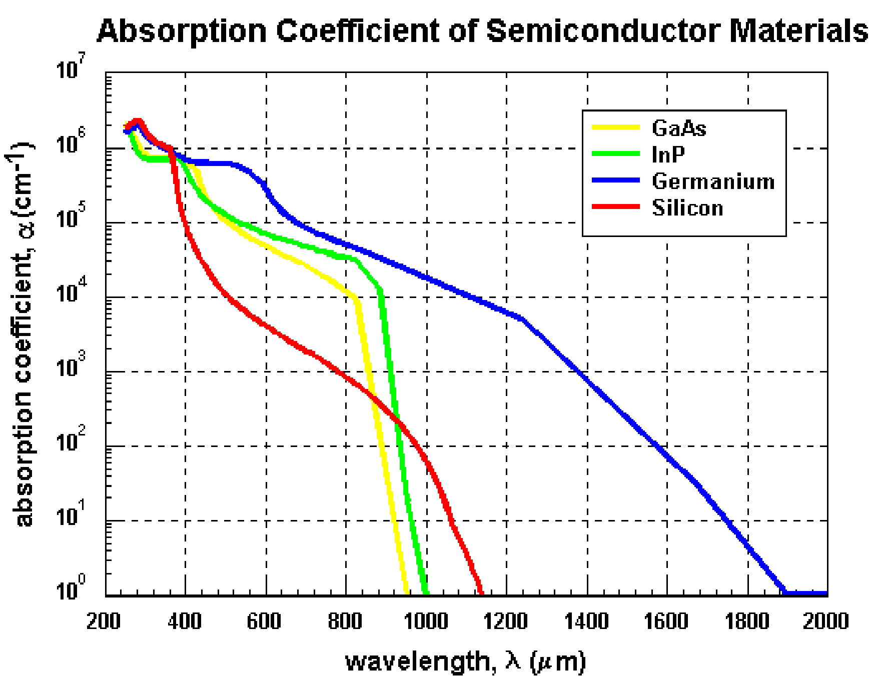
$$(h\varpi - E_G)^{1/2}$$

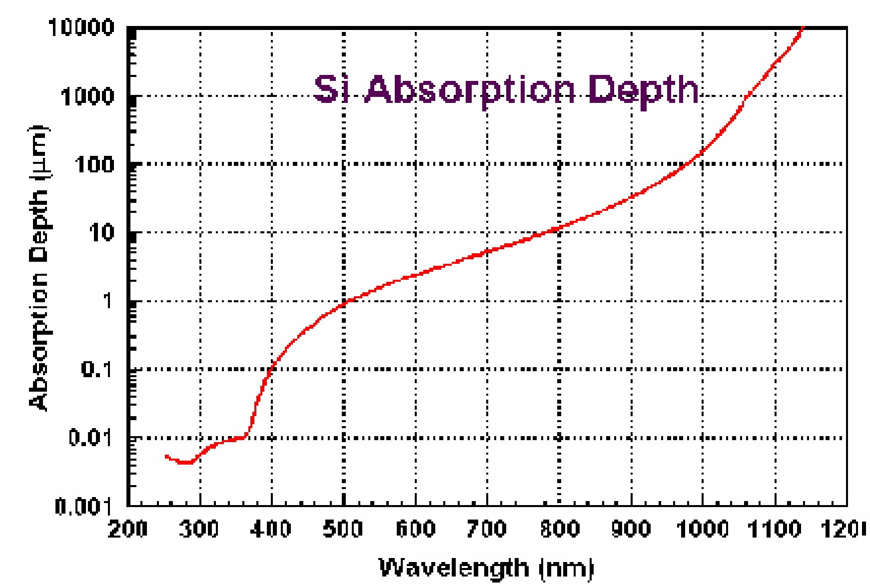
- **Temperature changes in a material cause a change in the band gap (E_G ↑ as T ↓), hence changing the absorption edge in a material.**



Generation: Absorption coefficient

- Direct band gap material generally have more rapid increase in absorption and larger α
- Absorption depth, $1/\alpha$, where intensity of light in semiconductor falls to 1/e, also commonly used.





Generation Rate

- Generation rate given by the number of photons absorbed on a material, and usually assumed to give alter the number of carriers in the energy bands.
- Number of photons at a given distance x into a material given by:

$$N_{ph} = N_s e^{-\alpha x}$$

Nph is the number of photons in the material
Ns is the number of photons at the surface
α is the absorption co-efficient and depends on λ
x is the distance into the material

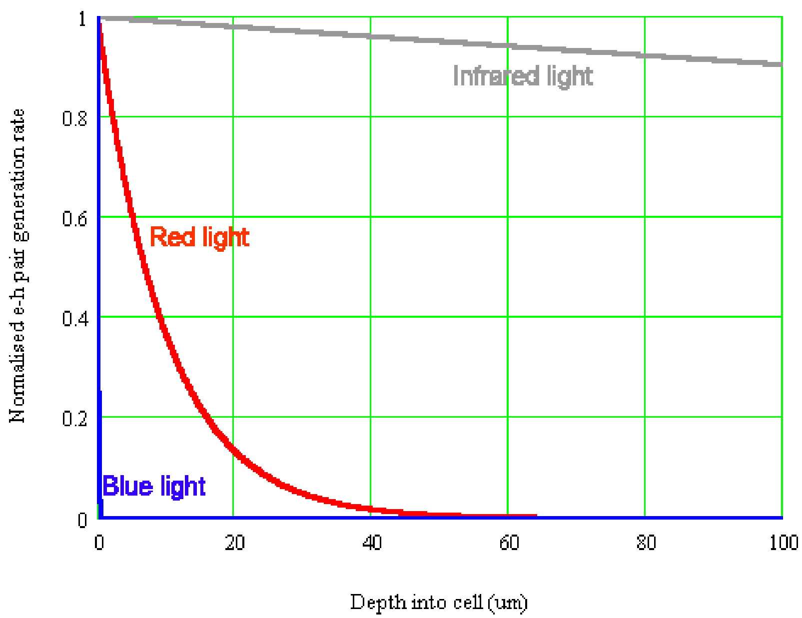
- Generation rate given by:

$$G = -\frac{dN_{ph}}{dx} = \alpha N_s e^{-ax}$$

Generation Rate

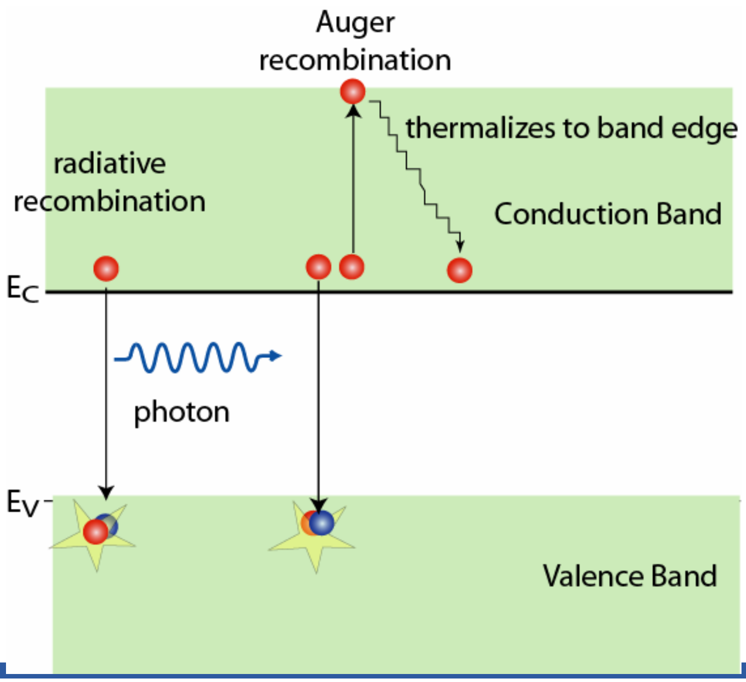
- Generation rate depends on the wavelength of incident light (different α) and also varies with position in the material.
- Large α means light absorbed close to surface, small α means light absorbed relatively uniformly in entire material.
- If x << 1/α, then generation can be assume constant.

$$G = \alpha N_s e^{-ax}$$



Recombination

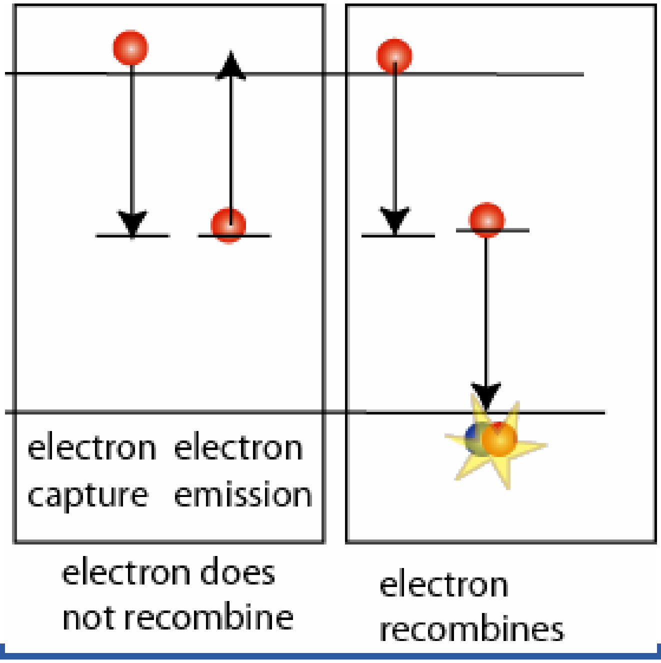
- Recombination is the inverse of absorption – any process in which an electron from the conduction band eventually resides in the valence band
- Recombination mechanisms: two significant fundamental processes: auger and radiative recombination.
- In radiative recombination, an electron directly combines with a hole in the conduction band.
- Requires a direct band material, where it is often the dominant process.



- In Auger recombination, a carrier recombines, but instead of emitting a photon, gives of its excess energy to another carrier in the same band, which then thermalises down to the its respective band edge.
- This process is the inverse of impact ionization
- Auger recombination is most important in heavily doped or heavily exited material

Recombination

- Defect recombination: a defect introduces an additional state into the forbidden band
- Recombination through defect is called Shockley-Read Hall Recombination (SRH recombination)
- SRH recombination is a two-step process: A carrier is trapped by an energy state in the forbidden region (introduced either thorough defects or through doping). If a hole moves up to the same energy state before the electron is thermally re-emitted into the conduction band, then it recombines.
- For energies close to either band edge, recombination is less likely.
- Energy levels near mid-gap are very effective for recombination
- SRH recombination dominates in indirect semiconductors



SRH Recombination

- Recombination processes are characterized by the minority carrier lifetime, which is the average time a minority carrier will take to recombine via a given process.
- Recombination calculated by:

$$\frac{dn}{dt} = c_n n p_T \qquad \frac{dp}{dt} = c_p p n_T$$

c is the capture co-efficient of the particular recombination process (i.e., how likely the process is to occur)
p_T, n_T is the number of empty states available for the carrier to go to.
n, p is the number of electrons or holes

$$R = \frac{dn}{dt} = \frac{dp}{dt} = \frac{np - n_i^2}{\tau_n(n + n_1) + \tau_p(p + p_1)}$$

n and *p* are the total electron and hole concentrations
n_i^2 is the intrinsic carrier concentration
τ_n and τ_p are the carrier lifetimes
n_1 and p_1 are the number of electrons and holes occupying trap energy E_T

- Under low level injection and using Δn=n-no, the above equation simplifies to:

in n-type material $$R = \frac{\Delta n}{\tau_n}$$

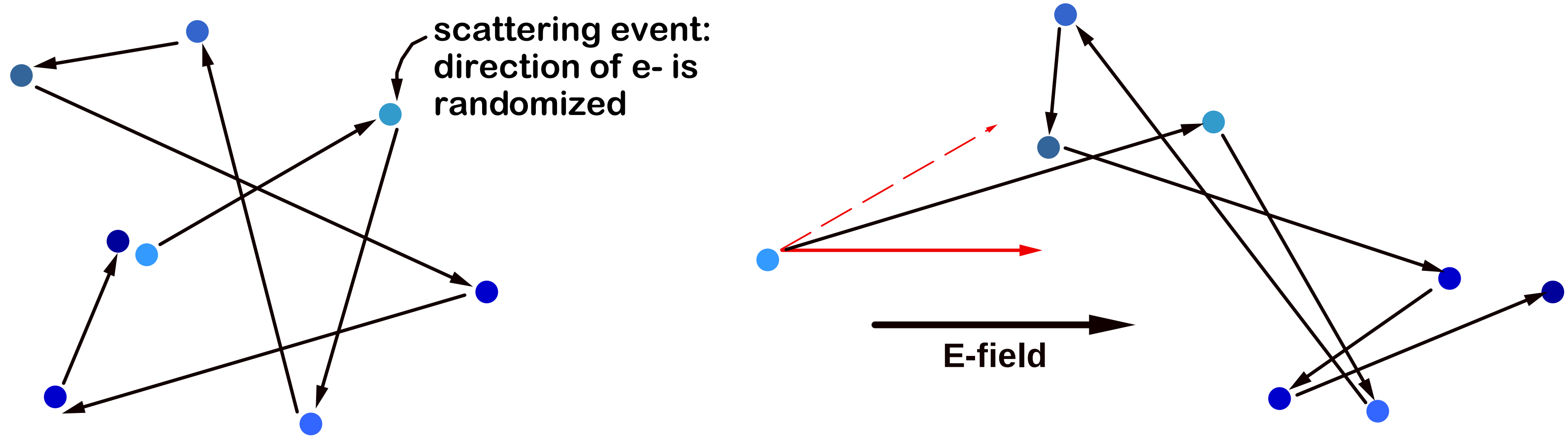
in p-type material $$R = \frac{\Delta p}{\tau p}$$

- The total recombination rate is given by: .

$$\frac{1}{\tau} = \frac{1}{\tau_{rad}} + \frac{1}{\tau_{SRH}} + \frac{1}{\tau_{aug}}$$

Transport

- We will consider two transport mechanisms: Drift and diffusion.
- Both these transport mechanisms depend on constant, random motion of electrons.
  - Electron moves in a given direction until it scatters due to an interaction with the crystal lattice.
- Drift transport: In the presence of an Electric field, a carrier movement due to the presence of the E-field is superimposed on the random motion.



Transport

- The mobility of the carriers depends on the mean time between scattering events.

$$\mu_n = \frac{qt}{m_n^*}$$

where t is the average time between scattering events and m is the effective mass

- Current due to electric field

$$J_n = -qnv_d = q\mu_n n\hat{E}$$
$$J_p = -qpv_d = q\mu_p p\hat{E}$$

$$J_{total} = J_n + J_p = q\left(\mu_n n + \mu_p p\right)\hat{E}$$
$$\sigma = \frac{1}{\rho} = q\left(\mu_n n + \mu_p p\right)$$

Transport

- Diffusive transport: occurs due to concentration gradients in carriers.

$$J_n = +qD_n \frac{dn}{dx}$$ for electrons and

$$J_p = -qD_p \frac{dp}{dx}$$ for holes.

$$D_p = \frac{kT}{q}\mu_p$$ for holes or

$$D_n = \frac{kT}{q}\mu_n$$ for electrons.

$$J_n = q\mu_n n\hat{E} + qD_n \frac{dn}{dx}$$

$$J_p = q\mu_p p\hat{E} - qD_p \frac{dp}{dx}$$