Defects in crystals

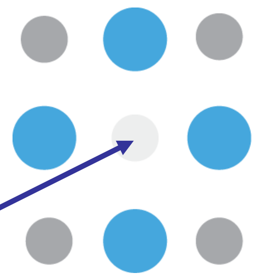
Ideal crystal:

electron's momentum $\hbar k$=const

F = 0 $v=\hbar k/m^*$ = const for small values of k (parabolic approximation)

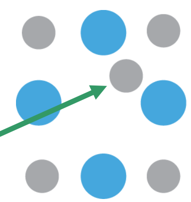
$\langle v \rangle \cong (3k_BT/m^*)^{0.5}$

Deviations from perfect lattice:



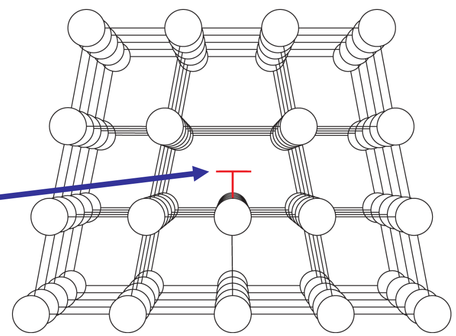
- lattice vibrations
- point defects

  a) intrinsic (vacancies, interstitials, antisites)



  a) impurities

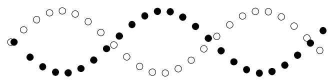
- line defects - dislocations



Lattice vibrations - phonons

acoustic phonon

optical phonon



$E_{fon} = \hbar\omega_f$ (~meV)

$p_{fon} = \hbar q$, $q_{max} = \pi/a$

$\lambda_{min} = 2a$ ⇒ $p_{fon\ max} = h/2a$

$$\mathbf{n_f} = \frac{1}{\exp\left\{\frac{\hbar\omega_f}{k_B T}\right\} - 1}$$

Bose-Einstein distribution:
number of phonons increases with temperature

Current transport

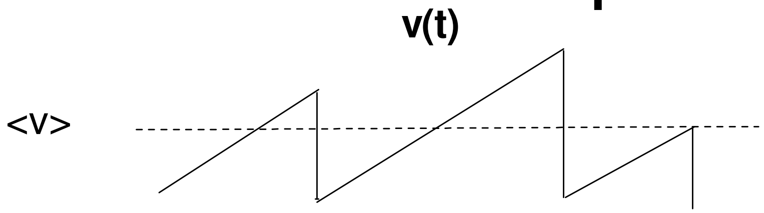
$$\vec{F} = e\vec{E} = \frac{d\vec{p}}{dt} = m^* \frac{d\vec{v}}{dt}$$

or

$$\vec{F} = e\vec{E} = \frac{d\vec{p}}{dt} = \frac{d(\hbar\vec{k})}{dt} = \hbar\frac{d\vec{k}}{dt}$$

$F_{ext}=0 \quad \rightarrow k = const$

collisions with lattice imperfections:



$F = eE$

$\langle v(t)\rangle = e\boldsymbol{E}\langle\tau\rangle/m^*$ $\quad\quad$ $\langle\tau\rangle$ - average time between collisions

drift velocity $v_d = \langle v\rangle = e\boldsymbol{E}\langle\tau\rangle/m^* = \mu\boldsymbol{E}$

$\mu = v_d/\boldsymbol{E} = e\langle\tau\rangle/m^*$ ***mobility, depends on lattice imperfections***

μ = *1-5000* cm^2/Vs; $\tau = 10^{-15}\text{-}10^{-12}$ *s*

Current transport

current density: $\mathbf{j=env_d}$

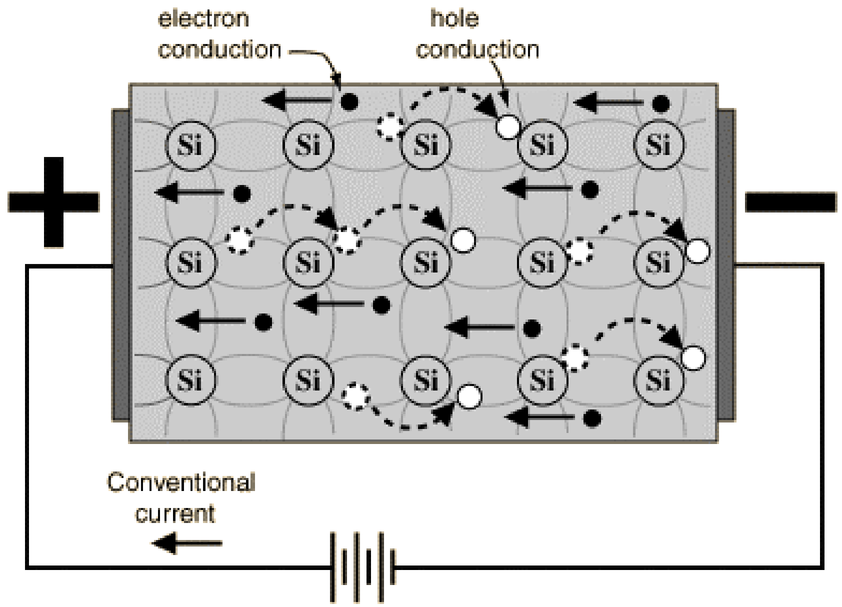
Ohm's law:

$j = \sigma E = en\mu_e$ *or* $j = ep\mu_h$

conductivity: $\sigma = en\mu_e$ ορ $\sigma = ep\mu_h$

$\mu = v_d / E$

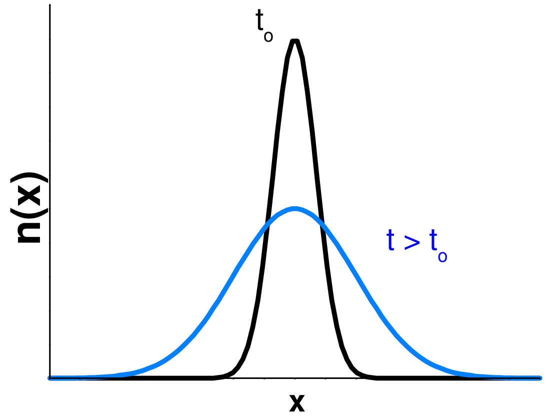
bipolar conductivity:
$\sigma = e(n\mu_e + p\mu_h)$



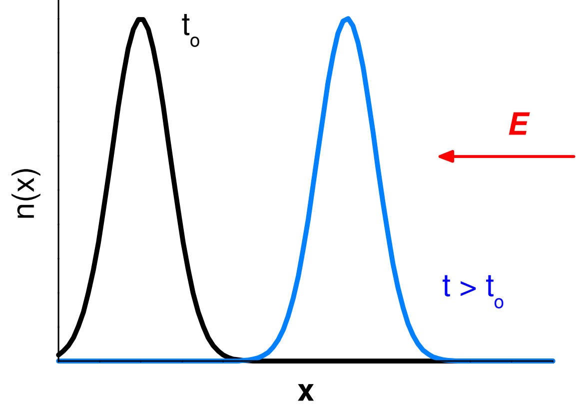
Drift current and diffusion current

$$\vec{j} = ne\mu\vec{\boldsymbol{E}} + eD\nabla n$$

diffusion constant: $D = \frac{k_B T}{e}\mu$ ***Einstein formula***



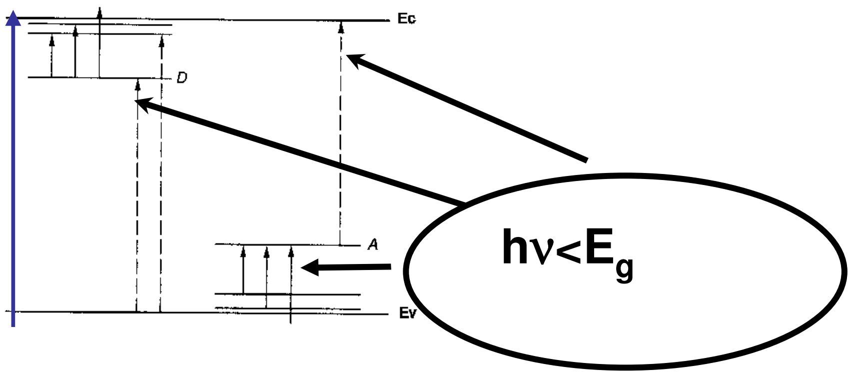
diffusion



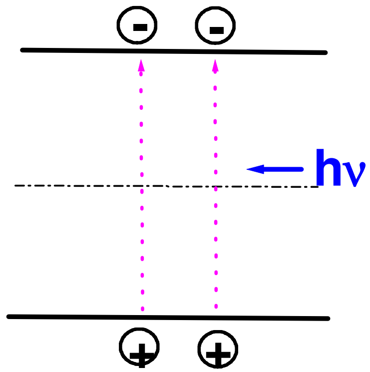
drift

Absorption of photons

band-to-band transition
$h\nu > E_g$
(fundamental absorption)



Only fundamental absorption leads to generation of free electron-hole pairs



photoconductivity

$\Delta\sigma = e(\mu_e \Delta n + \mu_h \Delta p)$

Absorption edge

$$\frac{dN}{dx} = -\alpha N$$

α- absorption coefficient

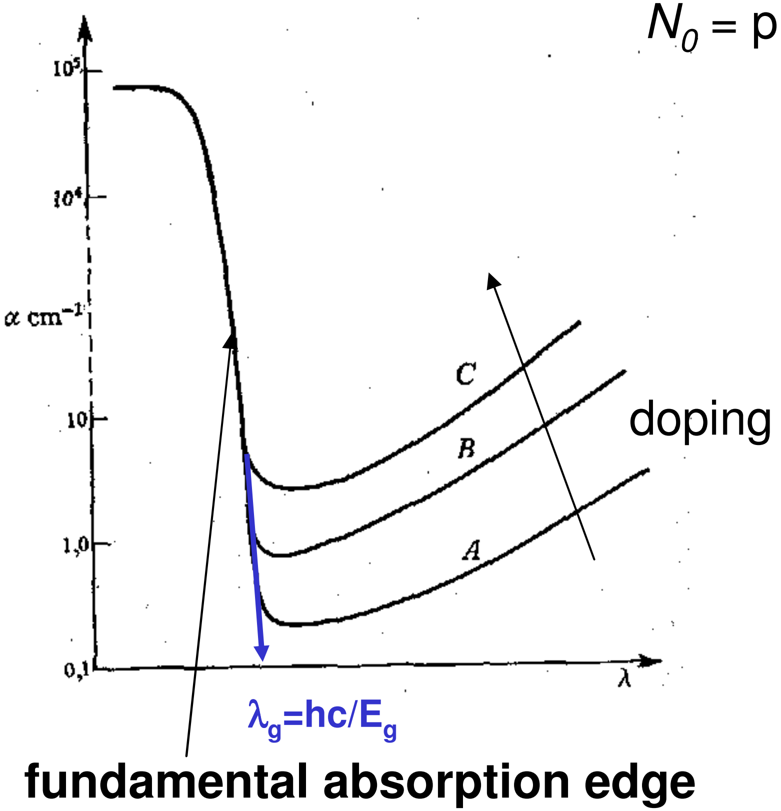
$$N = N_o e^{-\alpha x}$$

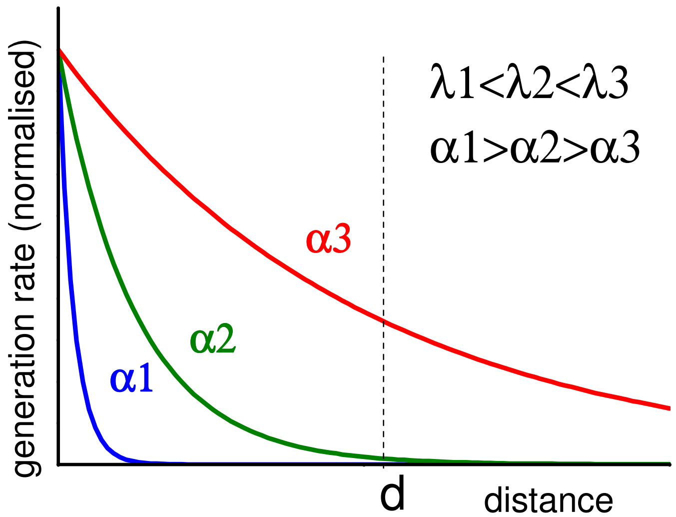
N(x) – photon flux

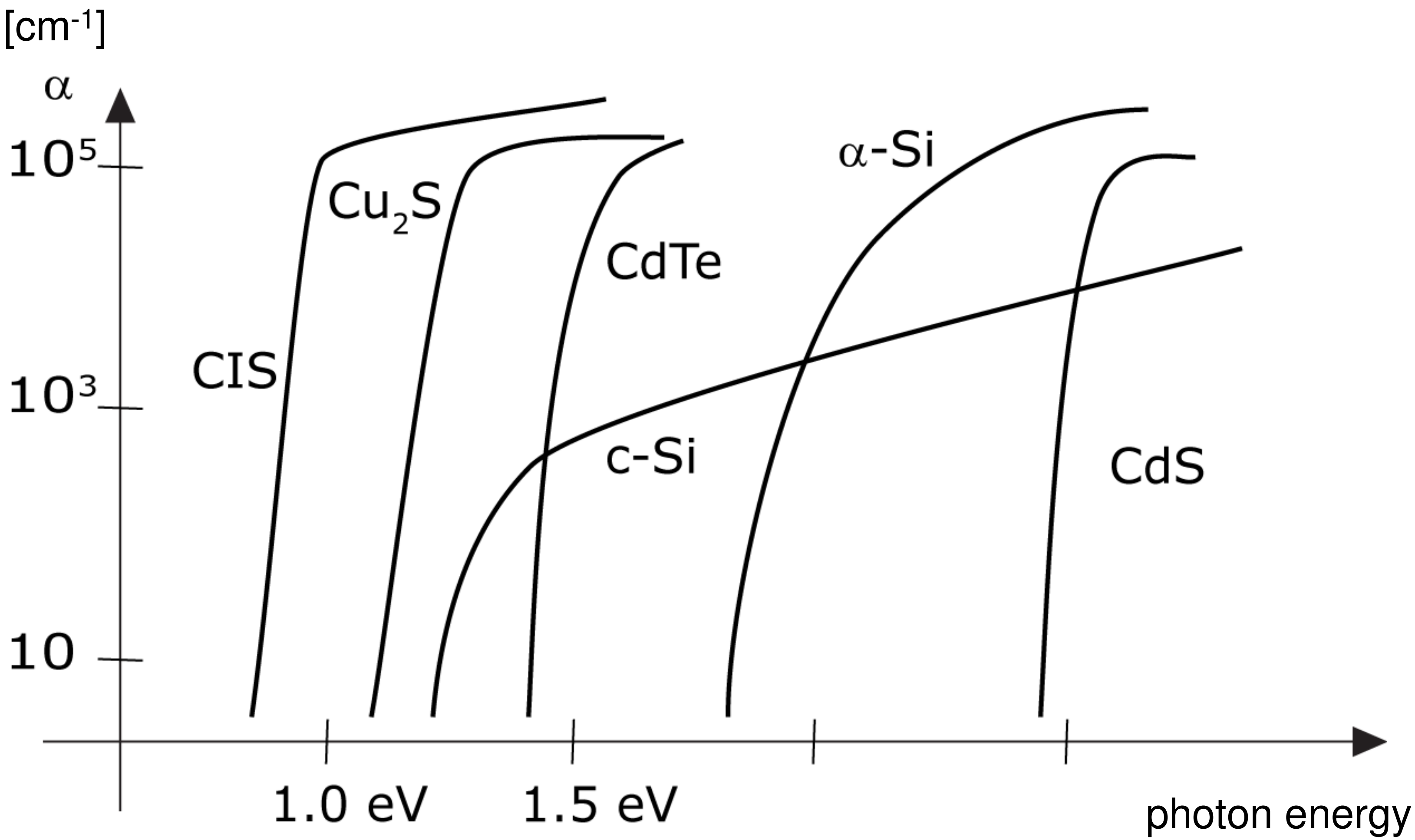
generation rate of electron-hole pairs

$$G = \alpha N_0 e^{-\alpha x}$$

N_0 = photon flux at the surface (photons/m²s)

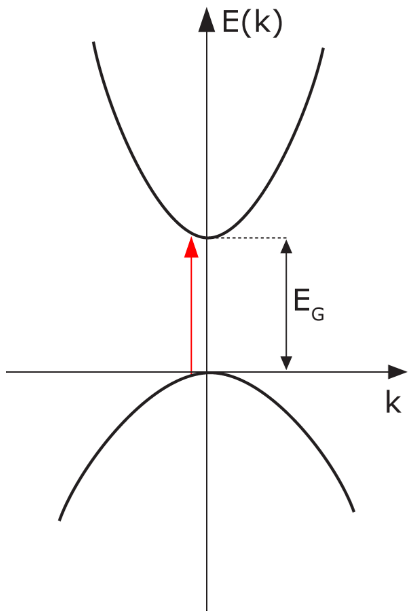





[cm-1]
α
10⁵
10³
10
CIS
Cu2S
CdTe
c-Si
α-Si
CdS
1.0 eV
1.5 eV
photon energy

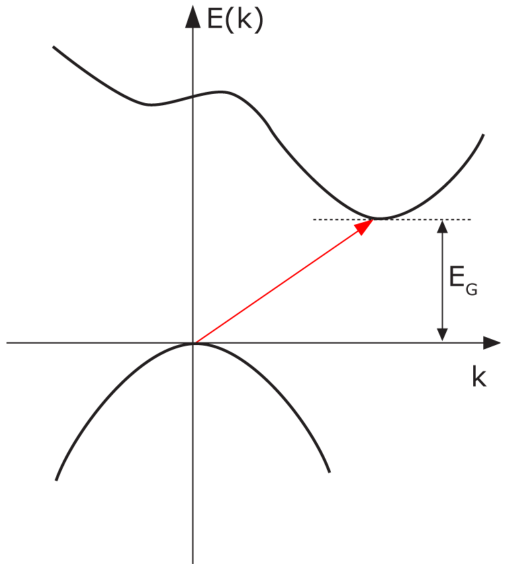
Fundamental absorption

direct transition



α (direct) >> α (indirect)

indirect transition



Conservation of energy and momentum:

$E_e + h\nu = E_e^*$

$k_e + k_{fot} = k_e^*$

$k_{fot} << k_e$

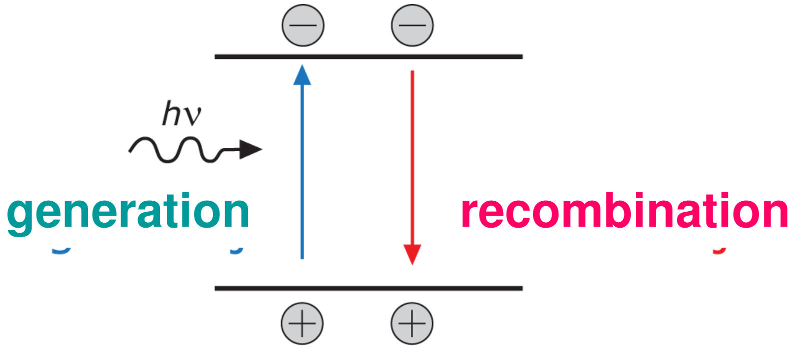
$k_e \approx k_e^*$

Conservation of energy and momentum :

$E_e + h\nu + h\omega_{fon} = E_e^*$

$k_e + k_{fon} \approx k_e^*$

Recombination



recombination: electron-hole pair disappears, energy is released through emission of photon (***radiative recombination***) or phonons (***non-radiative recombination***, often via defect centers)

$$\frac{\partial n}{\partial t} = G - R$$

$$R = \frac{(n - n_o)}{\tau} = \frac{\Delta n}{\tau}$$

e,h

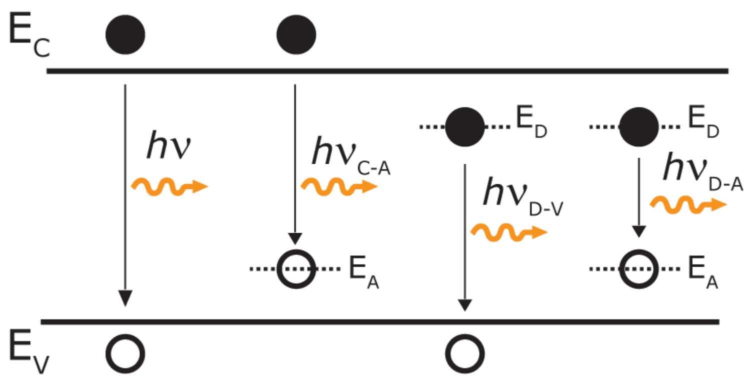
$$G = 0: \quad \Delta n(t) = \Delta n\ (0)\ \exp\ (-t/\tau)$$

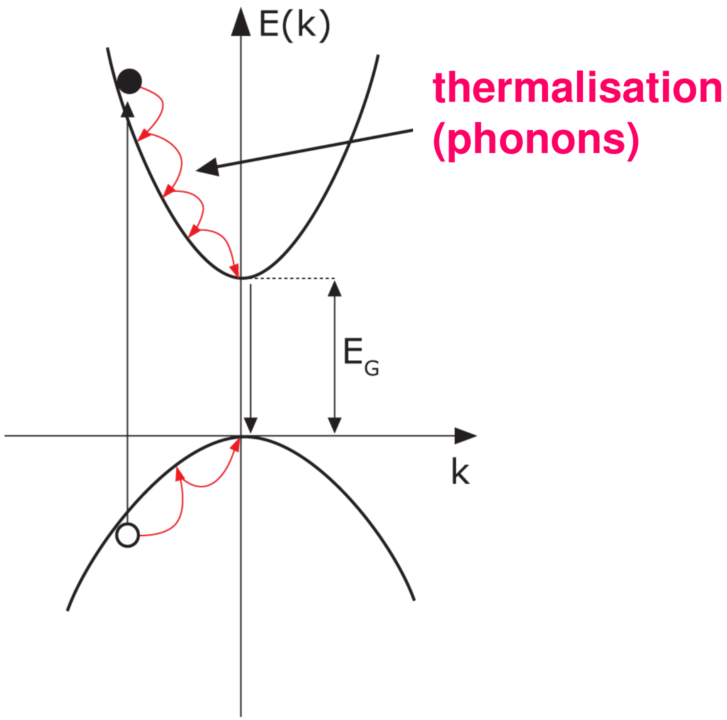
τ– lifetime of non-equilibrium carrier
how long it lives after generation before recombination,

steady-state under constant ilumination

$$\Delta n = \Delta p = G\tau \propto \alpha I_o \tau$$

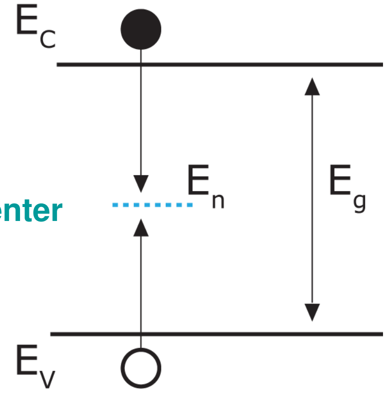
Radiative recombination





thermalisation – much faster process than photon emission

Non-radiative recombination



Recombination via defect states (Shockley-Read-Hall recombination)

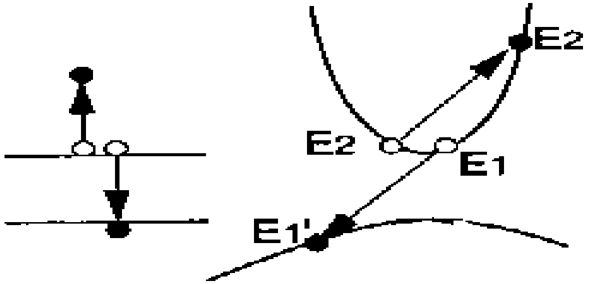
life-time of non-equilibrium carrier in case of SRH recombination

$$\tau_{e,h} = 1/\sigma_{e,h} v_{th} N_t$$

$\sigma = 10^{-20}$–10^{-12} cm^2 – capture cross section

N_t – concentration of defects

Auger recombination



energy of recombining electron (hole) transferred to another electron (hole) then realesed through thermalisation

$$\frac{1}{\tau_{bulk}} = \frac{1}{\tau_{Band}} + \frac{1}{\tau_{Auger}} + \frac{1}{\tau_{SRH}}$$

Nonequilibrium state

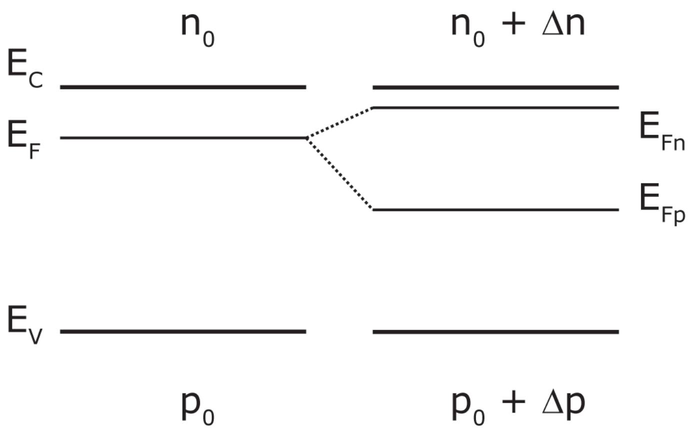
$n \neq n_o$; $f \neq f_o$; $np \neq n_i^2$

quasi-Fermi level E_F*

$$n = N_c \exp\left\{-\frac{E_c - E_{Fn}^*}{k_B T}\right\}$$

$$p = N_v \exp\left\{-\frac{E_{Fp}^* - E_v}{k_B T}\right\}$$

$$E_{Fn}^* \neq E_{Fp}^*$$



Continuity equation

(conservation of charge)

$$\frac{\partial \rho}{\partial t} + \nabla \vec{J} = 0$$

$$\frac{\partial n}{\partial t} = \frac{1}{e}\frac{\partial J_n}{\partial x} + G_e - R_e$$

$$\frac{\partial p}{\partial t} = -\frac{1}{e}\frac{\partial J_p}{\partial x} + G_h - R_h$$

G – generation velocity
R – recombination velocity

Diffusion length

$$j = ne\mu \boldsymbol{E} + eD\nabla n$$
$$D = \frac{k_B T}{e}\mu$$

+

$$\frac{\partial n}{\partial t} = \frac{1}{e}\frac{\partial J_n}{\partial x} + G_e - R_h$$

⇓

if G_e=0

$$0 = \mu_e E \frac{\partial \Delta n}{\partial x} + D_e \frac{\partial^2 \Delta n}{\partial x^2} - \frac{\Delta n}{\tau_e}$$

$$E = 0: \quad \Delta n = n_o \exp\left\{-\frac{x}{L_d}\right\}$$

$$\text{diffusion length}: \; L_D = \sqrt{D_{e,h}\tau_{e,h}}$$

Diffusion length – how far a carrier diffuses before it recombines

100 nm $< L_D <$ 100 μm