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Part 4: Quasi-Equilibrium Transport

Q: How charge carriers flow when subject to external excitation?

Topics: Fermi-level in equilibrium, Quasi-Fermi levels, Drift and diffusion, Generation and recombination and carrier continuity.

EE5181: Semiconductor devices

EE, IIT Hyderabad

Shubhadeep B (shubhadeep@ee at iith)

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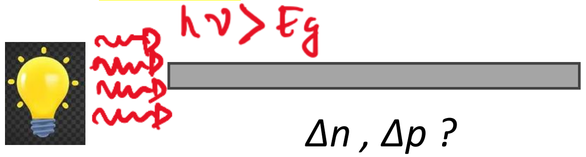
Si slab illuminated by light: Beyond thermal equilibrium

Q1) Excess Carriers, *Δp,n* (t)

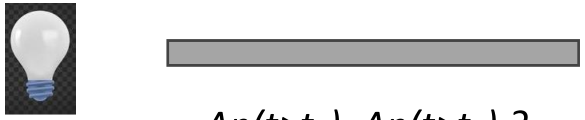
$n_0 = N_d = 10^{15}$, $p_0 = 10^5$
($np = n_i^2$) – Thermal Equ.

Case1: light ON at $x = 0$, t=0



Δn , Δp ?
Excess carrier "Generation"

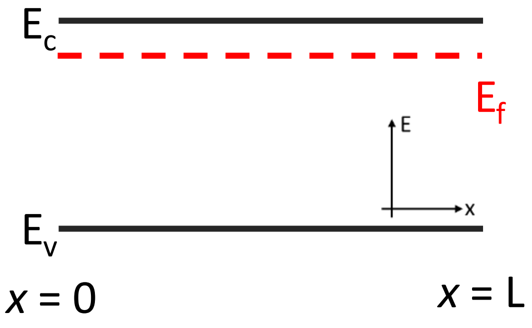
Case2: Bulb OFF, $t = t_1$



$\Delta n(t>t_1)$, $\Delta p(t>t_1)$?
Excess carrier "Recombination"

Topic 1: Generation & Recombination

Q2) Band Diagram, E_f?



Band Diagram?

Let's consider $\Delta n = 10^{14}$ Δp=?
$\Delta p = 10^{14}$ (e-h pairs)
Now, $n = n_0 + \Delta n = 1.1\text{x}10^{15}$
$p = p_0 + \Delta p \sim 10^{14}$

$np >> n_i^2$ Position of E_f?

Fermi-level picture insufficient for non-Equilibrium!

Topic 2: Quasi-Fermi Levels

Q3) Do the Excess carriers move in the slab *Δp,n* (x)?

$J_{drift} = \sigma E$, here $E = 0$
Therefore $J_{net} = 0$ No!

Spatial distribution of carriers

x = 0	*x = L*
n = *$1.1\text{x}10^{15}$*	n = *10^{15}*
p = 10^{14}	p = 10^5

Huge Spatial Gradient in *p* -> $\frac{dp}{dx}$

In nature: molecules diffuse from higher to lower concentration

{diffusion current}
$J_{p,diff} \propto dp/dx$

Topic 3: Drift and Diffusion

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Excess carrier "Generation"

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$\Delta n(t>t_1)$, $\Delta p(t>t_1)$?

Excess carrier "Recombination"

Topic 1: Generation & Recombination

Q2) Band Diagram, E_f?

E_c

E_f

E

x

E_v

$x = 0$ $x = L$

Band Diagram?

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e- e- e- e- e- e- e- e-
e- e- e- e- e- e- e- e-

E_c

E_v

h+ h+ h+ h+ h+ h+ h+ h+

Ideal Conditions:
Only Diffusion

e- e- e- e- e- e-
e- e- e- e- e- e-

E_c

E_v

h+ h+ h+ h+ h+ h+

Real Conditions:
Diffusion + Recombination
How to account? Charge conservation

Topic 3: Drift and Diffusion

Topic 4: Carrier Continuity

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Excess Carrier Generation and Recombination

Ideally:

In reality, Traps makes things more complex

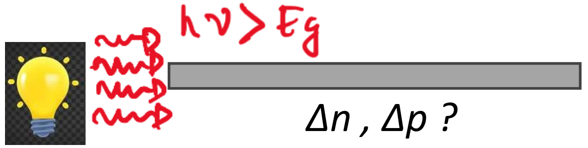
Generation: Breaking of bonds in VB: e-h+ creation, e- promoted to CB {2 free carriers generated}
Recombination: free e- in CB "drops" to VB, combines with a hole {2 free carriers annihilated}

Q: At thermal equilibrium: generation/recombination?

A: Yes! $R_{th} = G_{th}$; $R_{th} \propto n_0 p_0$ {equilibrium carr. conc. product} → Why??

$R_{th} = \alpha_R n_0 p_0 = \alpha_R n_i^2 = G_{th}$; R_{th} / G_{th} {Recomb/generation rates} $= \frac{d(P,N)}{dt}$

Back to our example:



Δn , Δp ?

Excess carrier "Generation"

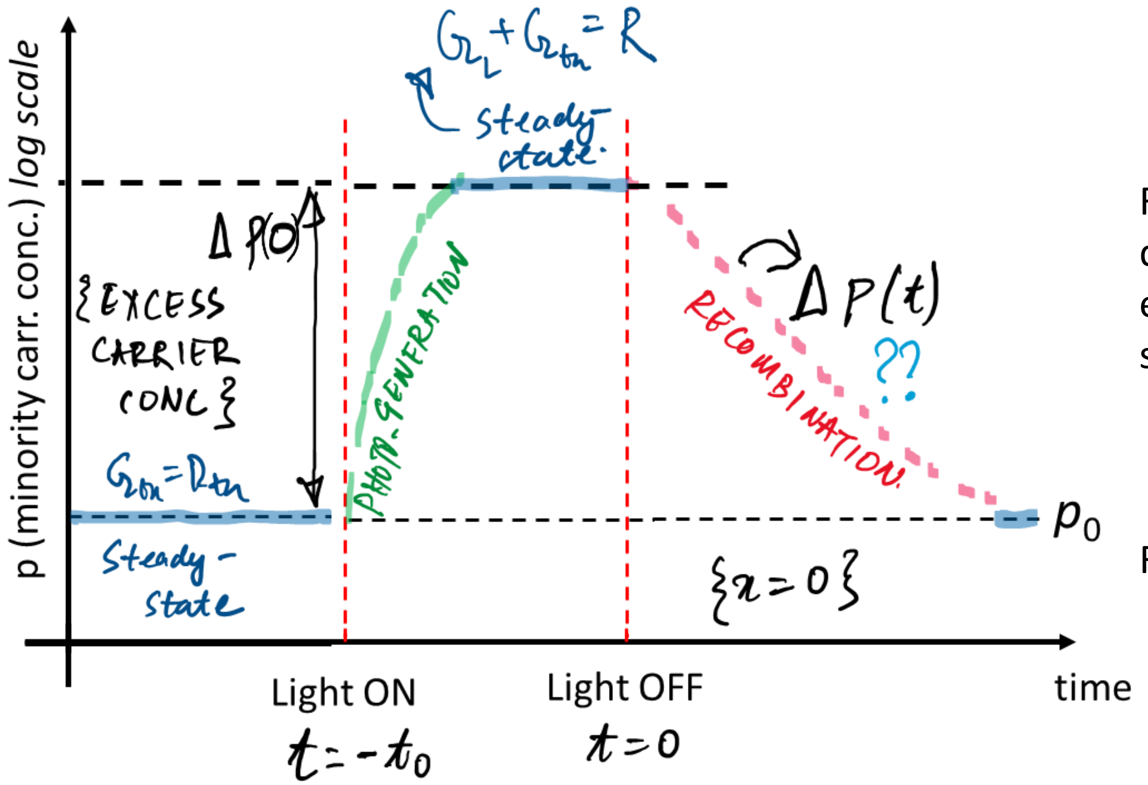
#1) fixed x=0
Δn(t), Δp(t)

#2) Minority carrier Injection approx.

$\Delta n, \Delta p \ll n_0$ → majority conc.
{excess carriers generated}

$10^{14}\ cm^{-3}$ $\quad 10^{15}\ cm^{-3}$

- $n(t) \approx 10^{15}\ cm^{-3}$
- $\boxed{p(t)}$



Remember we are dealing with dynamic equilibrium in steady state:

$$\frac{d(P,N)}{dt} = 0$$

$R_{net} = G_{net}$

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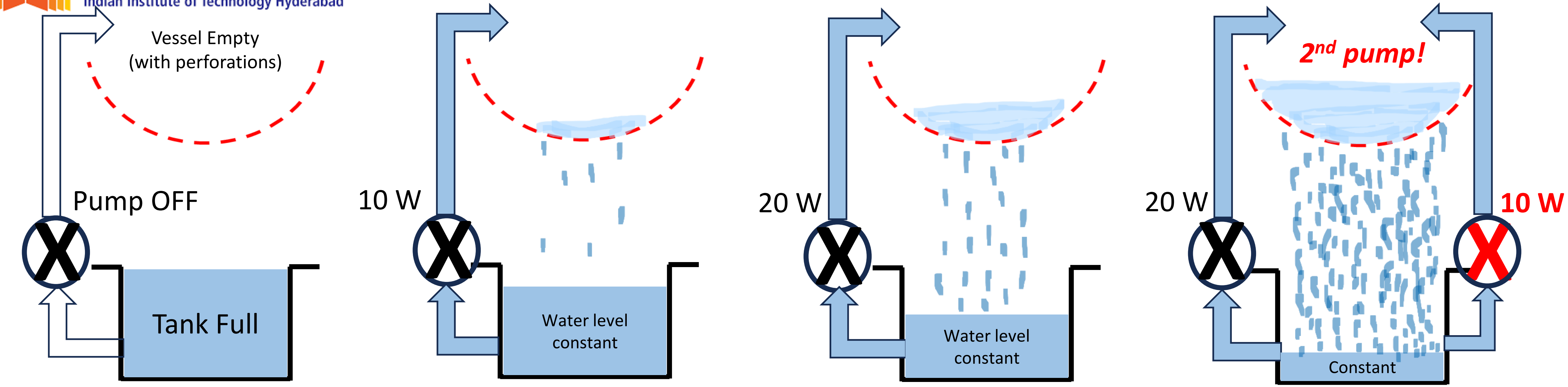
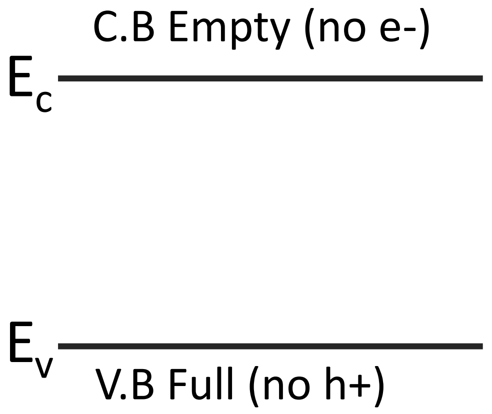
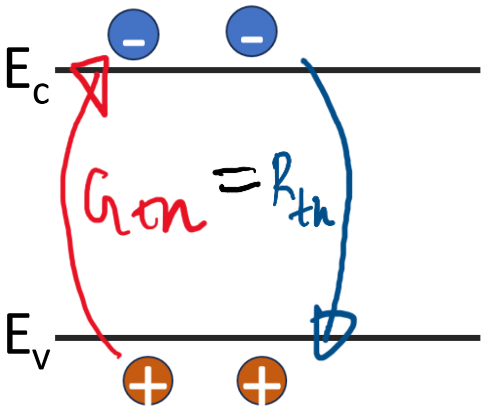
Dynamic Equilibrium: Perforated vessel, Tank and water pump analogy



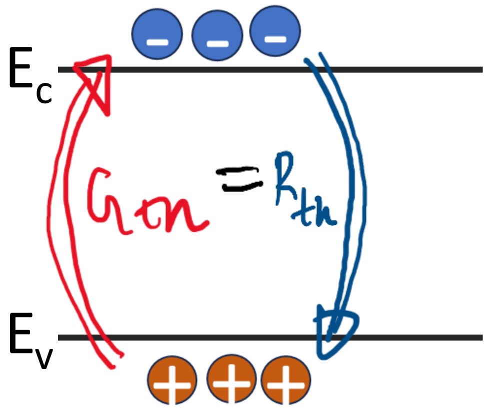
T = 0 K – Static Equilibrium
(No Generation/Recomb)



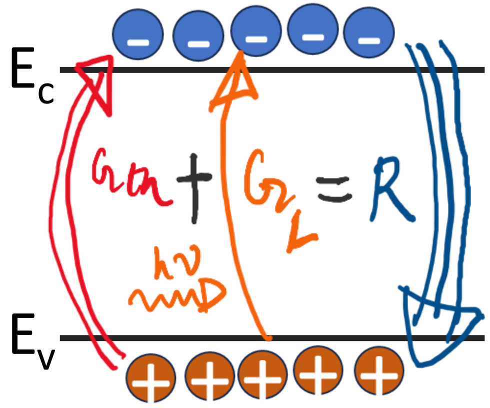
@Dynamic Equilibrium
T_1 K [R_{th} (T_1) = G_{th}(T_1)]



@Dynamic Equilibrium
$T_2 > T_1$ [R_{th} (T2)= G_{th}(T2) > G_{th}(T2)]



@Dynamic Equilibrium (with light)
$G_L + G_{th} = R$



Credits: Prof. M.R. Shenoy (IIT Delhi)

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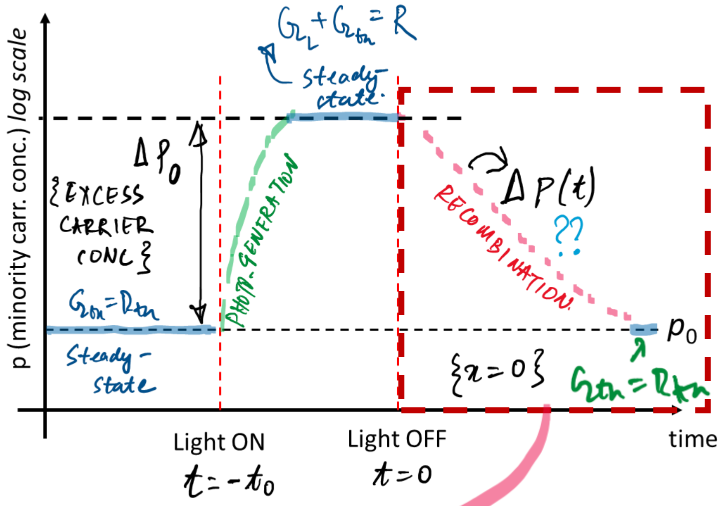
Minority Recombination lifetimes (τ)



$$R_{net} = -\frac{d\,\Delta p(t)}{dt} = \underbrace{\alpha_R\, n(t)\, p(t)}_{\text{new Recomb due to excess carrier} \to G_L} - \underbrace{\alpha_R\, n_0 p_0}_{R_{th}\ \text{always present.}}$$

Remember,

$n(t) \to \Delta n(t) + n_0$ {Total carr @t}

$p(t) \to \Delta p(t) + p_0$

$$n(t)\,p(t) = \cancel{\Delta n(t)\,\Delta p(t)} + \cancel{p_0\,\Delta n(t)} + \boxed{n_0\,\Delta p(t)} + \cancel{n_0 p_0}$$

Considering, $n_0 > \Delta p(t) = \Delta n(t) \gg p_0$

$$R_{net} = \alpha_R\, n_0\, \Delta p(t)$$

$$-\frac{d\,\Delta p(t)}{dt} = \alpha_R\, n_0\, \Delta p(t)$$

$$\Delta p(t) = \Delta p(0)\, e^{-\alpha_R n_0 t}$$

$$= \Delta p(0)\, \exp\left(\frac{-t}{1/\alpha_R n_0}\right)$$

$$\tau_p = \frac{1}{\alpha_R n_0}$$ {minority recombination life time}

$$\therefore\ \boxed{R_{net} = -\frac{d\,\Delta p(t)}{dt} = -\frac{\Delta p(t)}{\tau_p}}$$

{For n-type material}

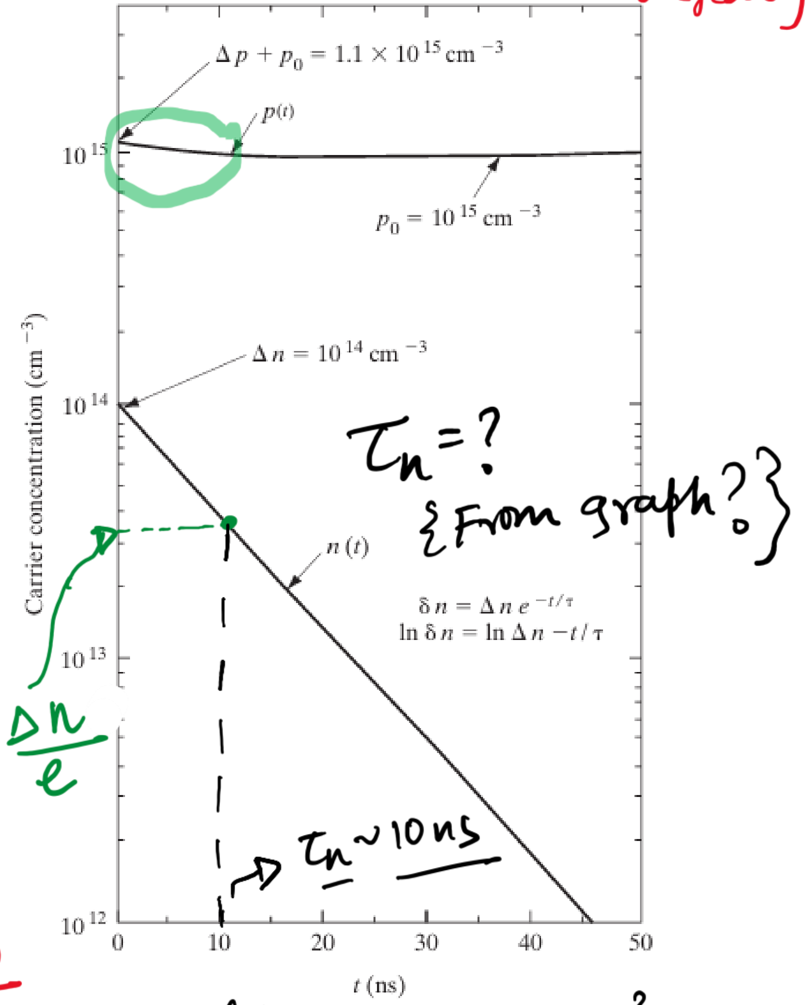
||ly for p-type material

$$\tau_n = 1/\alpha_R p_0 \to R_{net} = \frac{-\Delta n(t)}{\tau_n}$$

Ex:- Recomb of excess carr.

p-type Si $\to p_0 = 10^{15}\,cm^{-3}$; $n_0 = 10^5\,cm^{-3}$

$\Delta n_0 = \Delta p_0 = 10^{14}\,cm^{-3}$ {low-level injection}



{Streetman Banerjee}

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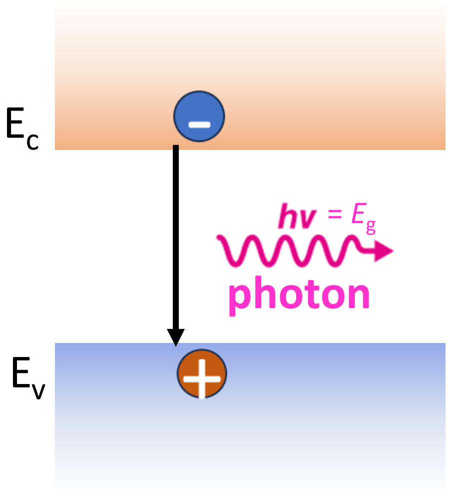
Overview of Physical Recombination mechanisms

1. Direct (Band to Band) vs ***Indirect*** (Trap Mediated) - different from direct/indirect semiconductors.

2. Radiative (energy emitted as E_g = hv) vs ***Non-Radiative*** (energy transferred to lattice or another carrier by phonons)

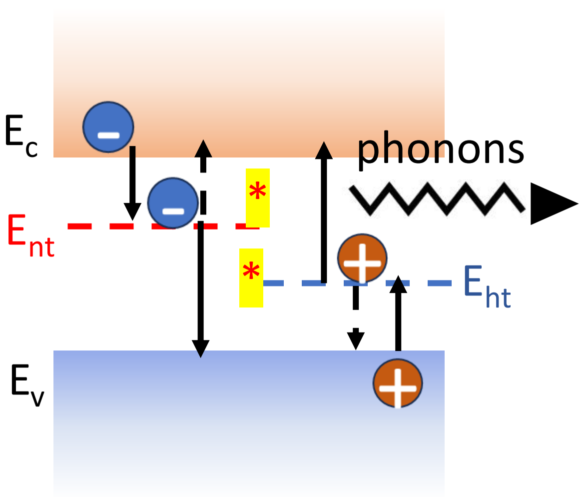
Direct-Radiative



Likely in defect free, direct band gap materials. (ex: GaAs)

Spatial and Energy Heterostructure Engineering to induce Direct Radiative recombination for LED/Laser

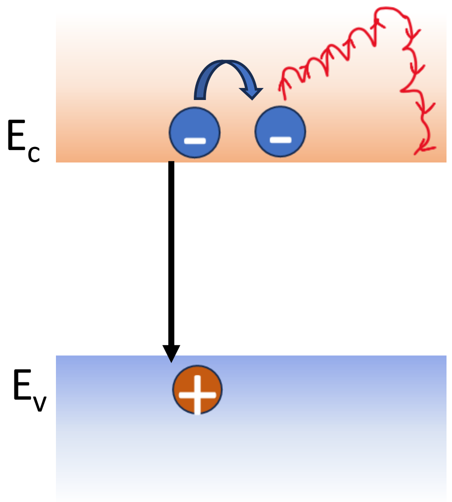
Indirect Trap Assisted Shockley Read Hall (SRH)



Likely in indirect band-gap, with mid-gap defects direct band gap materials. (example: Si, Ge)

Terrible for solar cells/optoelectronics and electronic applications.
Why? *immobilized carriers in trap states

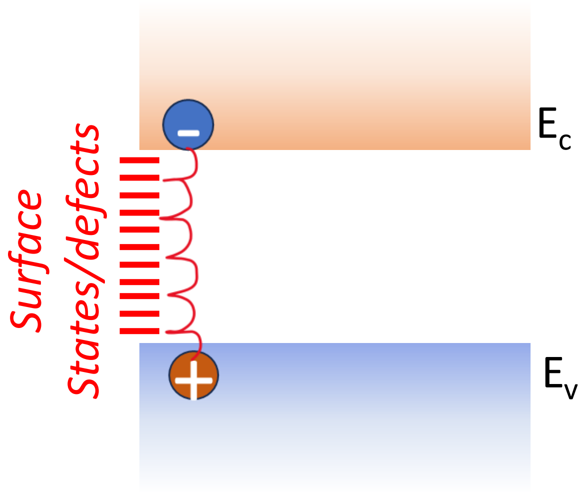
Auger, non-radiative (Direct/Indirect)



3- particle energy from recomb transferred to e-/h+, which eventually thermalizes)

Rare, mostly in high carrier concentrations and/or majority injection.

Surface (non-radiative)



Recombination mediated by surface states

Big problem for most devices especially solar cells. Mitigated by Surface passivation

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$x = 0$ *Silicon Block* $x = L$

$n_0 = N_d = 10^{15}$, $p_0 = 10^5$
($np=n_i^2$) – Thermal Equ.

Case1: light ON at $x = 0$, t=0

$h\nu > E_g$

Δn , Δp ?
Excess carrier "Generation"

Case2: Illuminated at $x = 0$, t = t_1

$\Delta n(t>t_1)$, $\Delta p(t>t_1)$?
Excess carrier "Recombination"

Topic 1: Generation & Recombination

Q2) Band Diagram, E_f?

E_c

E_f

E

x

E_v

$x = 0$ $x = L$

Band Diagram?

Let's consider $\Delta n = 10^{14}$ Δp=?
$\Delta p = 10^{14}$ *(e-h pairs)*
Now, $n = n_0 + \Delta n = 1.1\text{x}10^{15}$
$p = p_0 + \Delta p \sim 10^{14}$

$np >> n_i^2$ *Position of* E_f?

Fermi-level picture insufficient for non-Equilibrium!

Topic 2: Quasi-Fermi Levels

Q3) Do the Excess carriers move in the slab $\Delta p,n$ (x)?

$J_{drift} = \sigma E$, here $E=0$
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Spatial distribution of carriers

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$n = 1.1\text{x}10^{15}$ $n = 10^{15}$

$p = 10^{14}$ p- diffusion $p = 10^5$

$J_{p,diff}$

Huge Spatial Gradient in p -> $\frac{dp}{dx}$

In nature: molecules diffuse from higher to lower concentration

{diffusion current}

$J_{p,diff} \propto dp/dx$

E_c e- e- e- e- e- e- e- e- e- e- e- e- e- e- e- e-

E_v h+ h+h+ h+ h+ h+ h+ h+

Ideal Conditions:
Only Diffusion

E_c e- e- e- e- e- e- e- e- e- e- e-

E_v h+ h+ h+h+ h+ h+

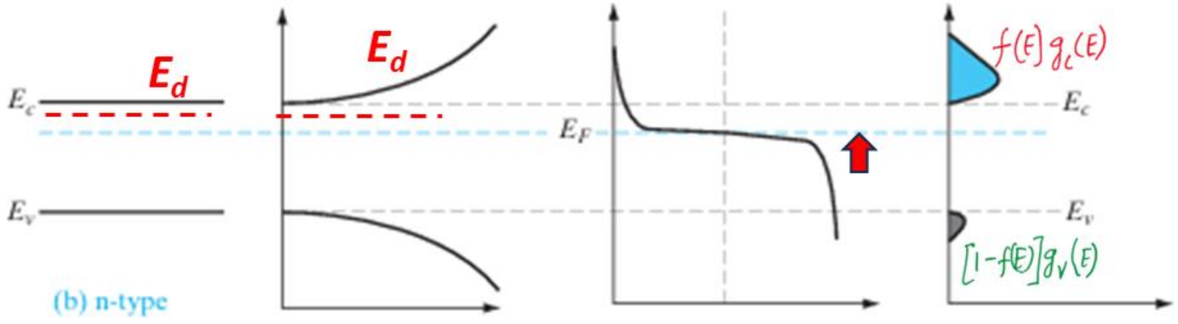
Real Conditions:
Diffusion + Recombination
How to account? Charge conservation

Topic 3: Drift and Diffusion

Topic 4: Carrier Continuity

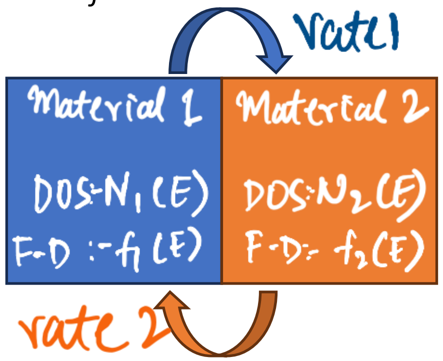
$E_f(x)$ and Thermal Equilibrium

Recall: E_f (E) slide ruler across ***band gap*** to find n,p @Thermal Equ.



What about E_f in band diagram i.e. E_f (x) ?

E_f invariance with x can be easily proved i.e. $\frac{dE_f}{dx} = 0$



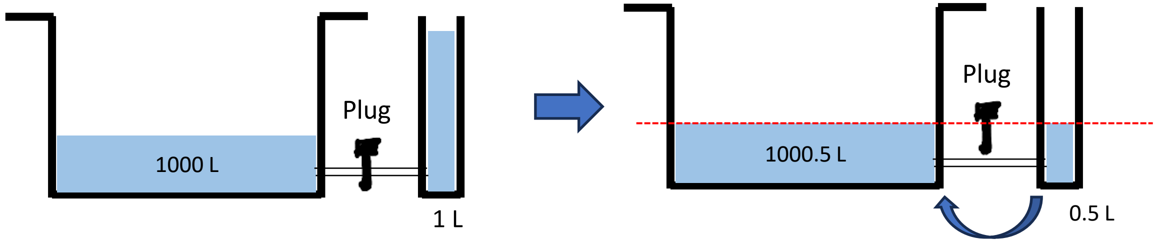
material 1/2 generic
n/p, similar/dissimilar
Semi-conductors OR metals.

Principle @ Thermal Equilibrium
↳ NO NET CHARGE TRANSFER
or $J_{net} = 0$

for any 'E' rate 1 = rate 2

Rate of charge transfer from region 1 ⇒ region 2 $\propto$ # filled states @ Reg. 1 × # empty states @ Reg. 2

@Equilibrium



When Plug is opened where will water flow from?

From test tube to reservoir! From filled to empty @ *h* P.E = mgh

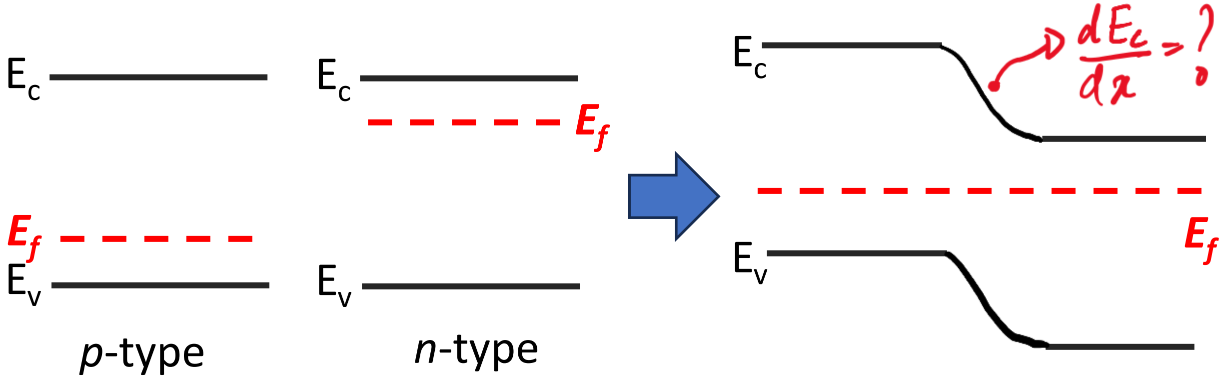
$\text{rate}_{1\to2}(E) \propto \underbrace{N_1(E) f_1(E)}_{\text{filled}} \times \underbrace{N_2(E)[1-f_2(E)]}_{\text{empty}}$

$\text{rate}_{2\to1}(E) \propto N_2(E) f_2(E) \times N_1(E)[1-f_1(E)]$

$\text{rate}_{1\to2}(E) = \text{rate}_{2\to1}(E) \} \Rightarrow f_1(E) = f_2(E);\ \boxed{E_{f_1} = E_{f_2}}$

@ Thermal equilibrium $E_{f_1} = E_{f_2} \Rightarrow dE_f/dx = 0$

Classic Example: p/n Junction @ Thermal Equilibrium



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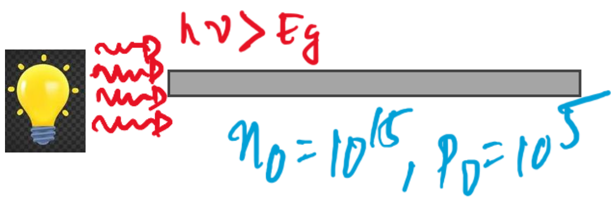
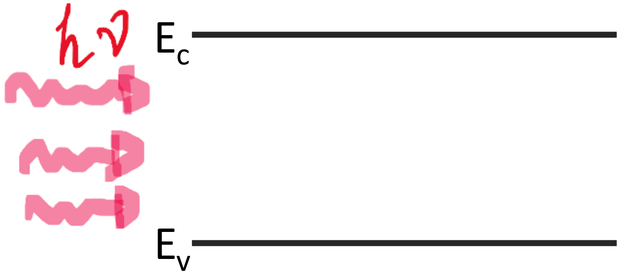
Beyond-thermal Equilibrium Case – Quasi Fermi-Levels

Revision: At Thermal Equilibrium – $np = n_i^2$ – Both *n,p* statistics described by single E_f

light ON at *x* = 0
NOT! Thermal Equlibrium!





x = 0

$\Delta n = \Delta p = 10^{14}$

$n = n_0 + \Delta n \simeq 1.1 \times 10^{15}$

$p = p_0 + \Delta p = 10^{14}$

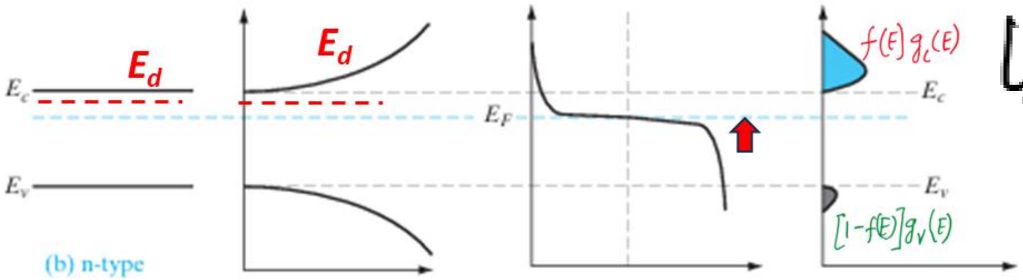
Note:- $np \gg n_i^2$

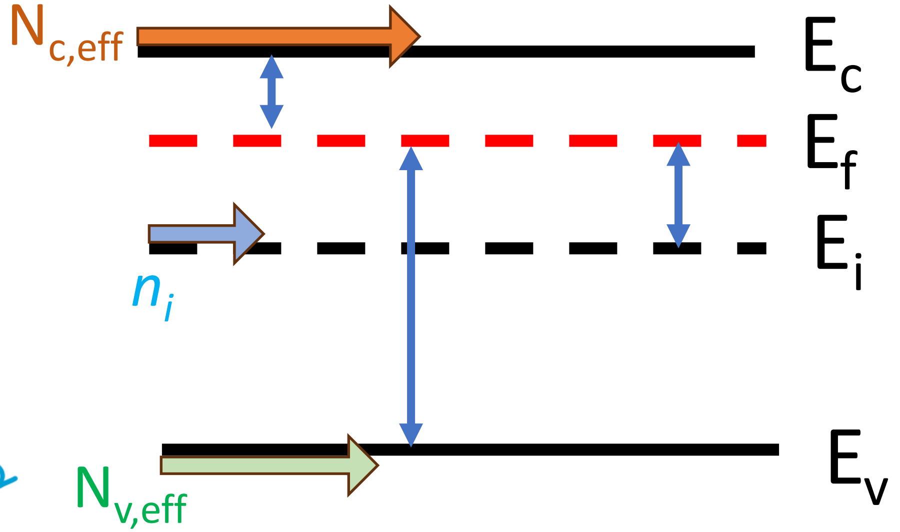
x = L
Very far away
No Excess carrier,

$n = n_0 ;\ p = p_0$

$np = n_0 p_0 = n_i^2$

Band Diagram, $E_F(x) = ?$





$\hookrightarrow n_0 = N_c \exp\left[\frac{-(E_c - E_F)}{k_B T}\right];$

$p_0 = N_v \exp\left[\frac{-(E_F - E_v)}{k_B T}\right]$

$\Rightarrow np = n_i^2$

Single 'E_F' sufficient to describe n & p.

$\hookrightarrow$ However, where $np \neq n_i^2$ {Beyond T.E.} SEPERATE / INDEPENDENT F-D stats & $E_{F,n/p}$ for n, p

"Quasi-Fermi Levels" – Similar, but not quite!

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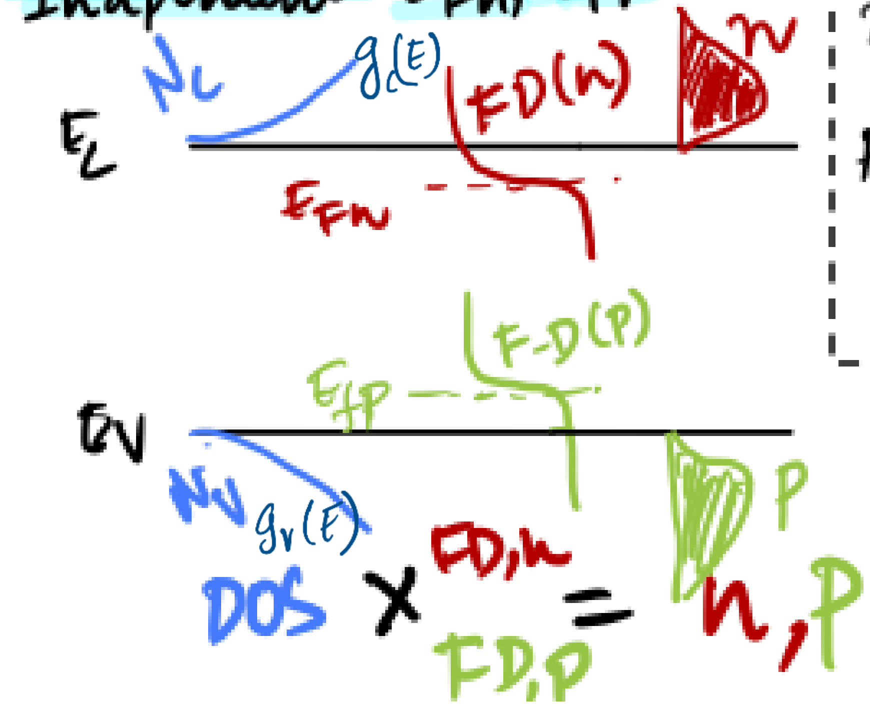
Beyond-thermal Equilibrium Case – Quasi Fermi-Levels

↳ However,
where $np \neq n_i^2$ {Beyond T.E.} SEPERATE / INDEPENDENT F-D stats & $E_{F,n/p}$ for n, p

"Quasi-Fermi Levels"

$E_{fn} \rightarrow$ QUASI- Fermi level for e^-
$E_{fp} \rightarrow$ QUASI - Fermi level for h^+

Independent E_{fn}, E_{fp}

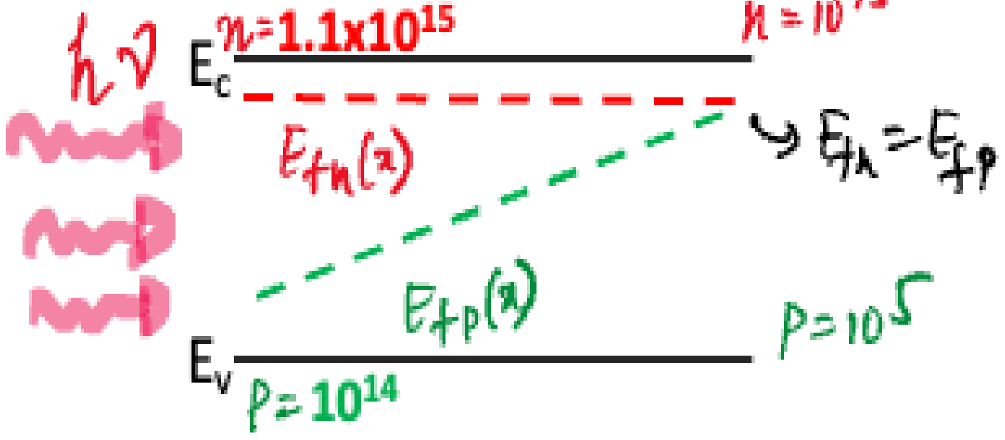


$$n(x) = N_c \exp\left[\frac{E_{fn}(x) - E_c}{k_B T}\right]$$
$$p(x) = N_v \exp\left[\frac{E_v - E_{fp}(x)}{k_B T}\right]$$
$$np = n_i^2 \exp\left[\frac{E_{fn} - E_{fp}}{k_B T}\right]$$

$E_{fn} > E_{fp} \Rightarrow np > n_i^2$ Generation, Injection

$E_{fn} < E_{fp} \Rightarrow np < n_i^2$ Recombination, Removal

E_{fn}, E_{fp} for our case?



** Note: Band Diagram NOT complete.

1) Charge distribution->E_{bi} gradient in E_c and E_v
2) Gradient in Quasi- Fermi Levels $d(E_{fn,p})/dx$ – What do they mean? – UP Next!

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Si slab illuminated by light: Beyond thermal equilibrium

Q1) Excess Carriers, *Δp,n* (t)

$x = 0$ *Silicon Block* $x = L$

$n_0 = N_d = 10^{15}$, $p_0 = 10^5$
($np = n_i^2$) – Thermal Equ.

Case1: light ON at $x = 0$, t=0

$h\nu > E_g$

Δn , Δp ?
Excess carrier "Generation"

Case2: Illuminated at $x = 0$, t = t_1

Δn(t>t₁), Δp(t>t₁) ?
Excess carrier "Recombination"

Topic 1: Generation & Recombination

Q2) Band Diagram, E_f?

E_c

E_f

E

x

E_v

$x = 0$ $x = L$

Band Diagram?

Let's consider $\Delta n = 10^{14}$ Δp=?
$\Delta p = 10^{14}$ *(e-h pairs)*
Now, $n = n_0 + \Delta n = 1.1\text{x}10^{15}$
$p = p_0 + \Delta p \sim 10^{14}$

$np \gg n_i^2$ *Position of* E_f?

Fermi-level picture insufficient for non-Equilibrium!

Topic 2: Quasi-Fermi Levels

Q3) Do the Excess carriers move in the slab *Δp,n* (x)?

$J_{drift} = \sigma E$, here $E = 0$
Therefore $J_{net} = 0$ No!

Spatial distribution of carriers

x = 0
n = *1.1x10¹⁵*
p = 10^{14}

x = L
n = *10¹⁵*
p = 10^5

p- diffusion

$J_{p,diff}$

Huge Spatial Gradient in *p* -> $\frac{dp}{dx}$

In nature: molecules diffuse from higher to lower concentration

{diffusion current}
$J_{p,diff} \propto dp/dx$

Topic 3: Drift and Diffusion

E_c e- e- e- e- e- e- e- e- e- e- e- e- e- e- e- e-

E_v h+ h+ h+ h+ h+ h+ h+ h+

Ideal Conditions:
Only Diffusion

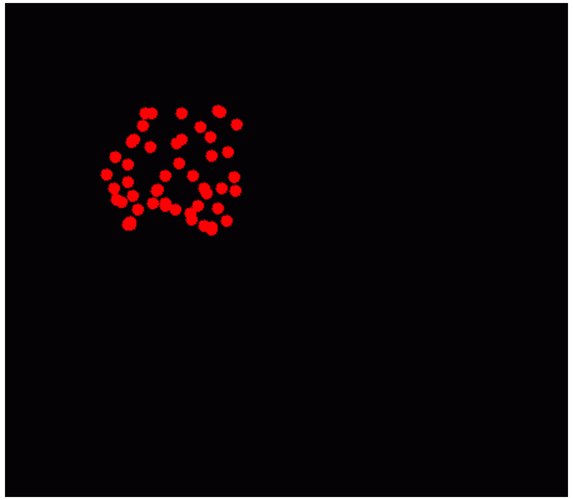
E_c e- e- e- e- e- e- e- e- e- e- e-

E_v h+ h+ h+ h+ h+ h+

Real Conditions:
Diffusion + Recombination
How to account? Charge conservation

Topic 4: Carrier Continuity

Diffusion of carriers - concentration gradient



Diffusion: random thermal motion of ‘free non-interacting’ particles – Continues till ‘uniform concentration achieved’

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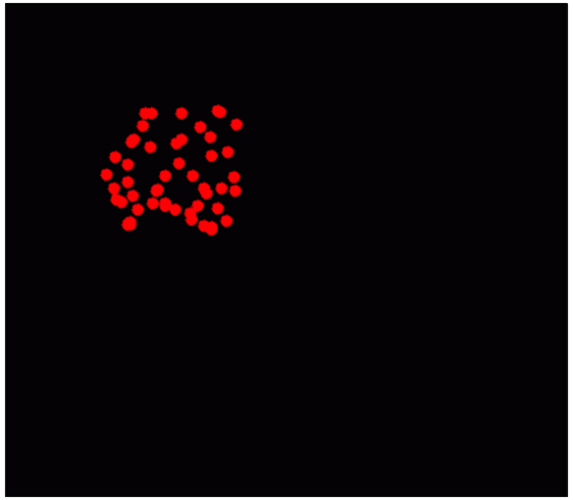
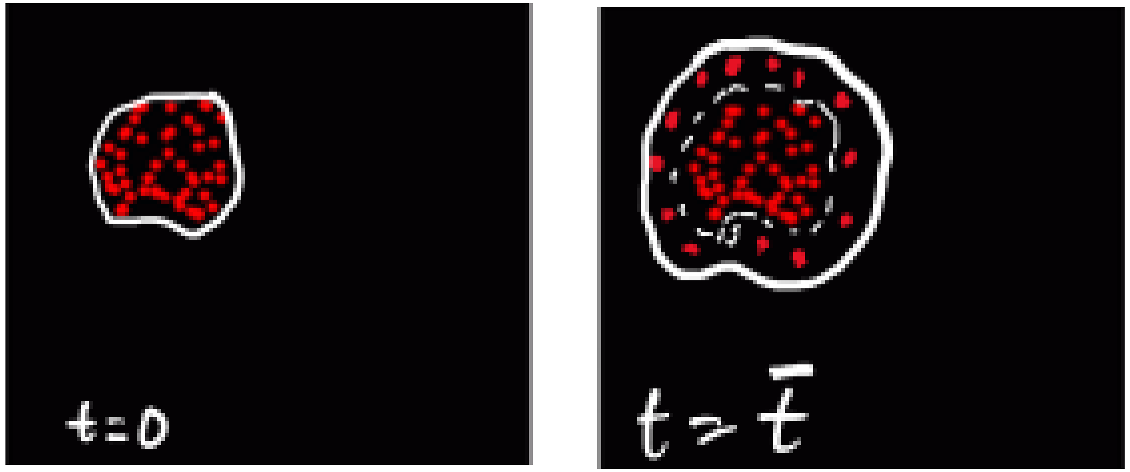
Diffusion of carriers - concentration gradient



Diffusion: random thermal motion of ‘free non-interacting’ particles – Continues till ‘uniform concentration achieved’

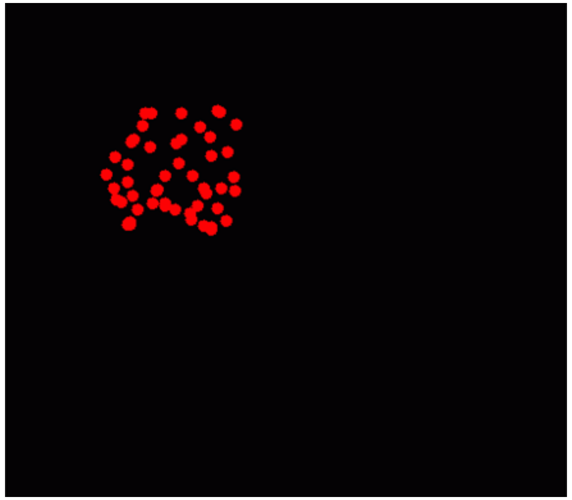


$\bar{t}$ {mean free time} → ‘t’ needed for 1/2 molecules move in & out of Vol_{init}.

$\bar{l}$ {mean free path} → average dist. moved by species before random collisions

Diffusion of carriers - concentration gradient

For Derivation see: Appendix 1



Can be easily derived,

flux $\rightarrow$ $\phi(x) \propto -\dfrac{d\,Conc}{dx}$ $\rightarrow$ conc

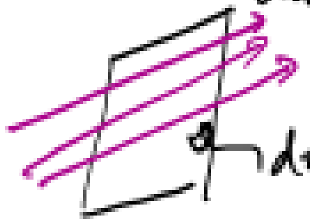
opposite to

$$\phi(x) = -D\,\frac{d\,Conc.}{dx}$$

Diffusion constant

1. $\phi(x) \Rightarrow$ flux $\dfrac{\text{rate of change}}{\text{unit area.}}$

$\{cm^{-2}s^{-1}\}$



dA. How many particles passed through dA per unit time.

2. D {Diffusion Coeff}
$-\ \bar{l}^2/2\bar{t} \rightarrow \{cm^2 s^{-1}\}$

Therefore for e^-

for $e^- \rightarrow \phi_n(x) = -D_n \dfrac{dn(x)}{dx}$

Remember, rate of flow charges per unit time $\rightarrow J(x)$ Therefore,

$$J_n^{diff}(x) = (-q)(-D_n\, dn(x)/dx)$$

-ve charge opp.

particles move opp. to gradient.

$$\boxed{J_n^{diff}(x) = q D_n \nabla n}$$

|||ly for h^+

$$\phi_p(x) = -D_p \frac{dp(x)}{dx}$$

$$\boxed{J_p^{diff}(x) = -q D_p \nabla p}$$

Net current: Drift-Diffusion formalism

J_{net} can have two sources (a) J_{drift} due to $\mathcal{E}_{ext}$ (b) J_{diff} due to spatial concentration gradient

Drift-Diffusion solver at the heart of all commercial TCAD simulators.

$$J_{net}(x) = J_n(x) + J_p(x) \; ; \; J_n(x) = \underbrace{q \mu_n n(x) \mathcal{E}(x)}_{\text{drift}} + \underbrace{q D_n \frac{dn(x)}{dx}}_{\text{diffusion}} \; ; \; J_p(x) = \underbrace{q \mu_p p(x) \mathcal{E}(x)}_{\text{drift}} - \underbrace{q D_p \frac{dp(x)}{dx}}_{\text{diffusion}}$$

<u>Drift Diffusion @ Thermal Equilibrium:</u>

Example: Exponentially doped semiconductor w/o any external excitation

$$\boxed{N_d(x) = N_{d0} e^{-x/\lambda}}$$

$x = 0$

$N_d = 10^{19}\ cm^{-3}$

$x = L$

$N_d = 10^{15}\ cm^{-3}$

Q1) Draw Band Diagram

Q2) Draw direction of drift diffusion for e- and h+

Q3) Draw J_{net}

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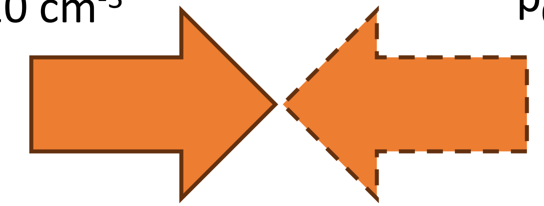
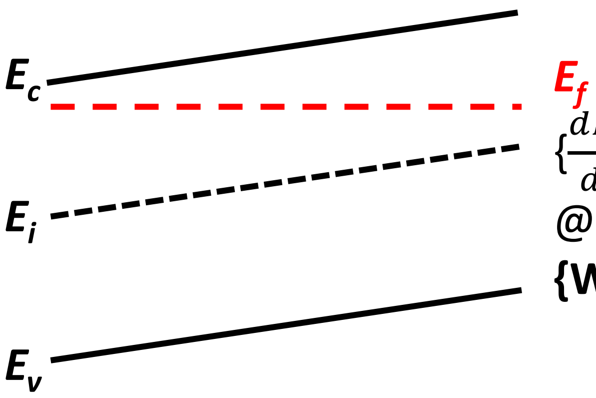


ϕ_n (DIFF) J_n (DIFF)

ϕ_p (DIFF) J_p (DIFF)

Why J_n(diff) >> J_p(diff)



$\{\frac{dE_f}{dx} = 0\}$
@T.E.

{Why is E_c and E_v vs. x Linear?}

$E_c(x) - E_f = kT/q \ln[n(x)/N_c]$

$n(x) \to e^{-x/\lambda}$

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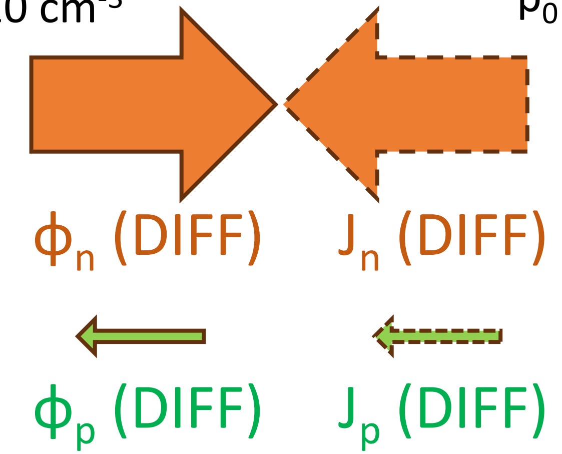

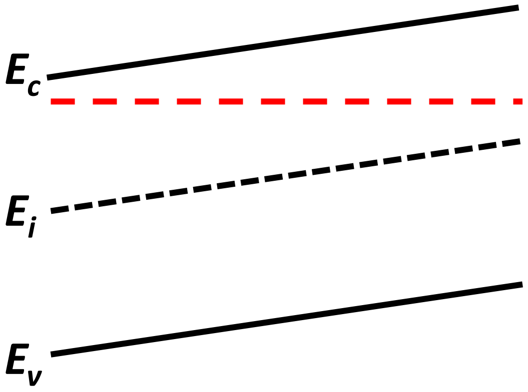

E_f $\{\frac{dE_f}{dx} = 0\}$
@T.E.

{Why is E_c and E_v vs. *x* Linear?}

$E_c(x) - E_f = kT/q \ln[n(x)/N_c]$

$n(x) \rightarrow e^{-x/\lambda}$

NOTICE @ $x = L$ 'n' conc. lower electrostatic Potential Energy higher!

NOTE :- Opposite for holes!

Remember gradient in 'V' $\Rightarrow \mathcal{E}$

$\mathcal{E}(x) = -\frac{dV}{dx} = \frac{-d(E_i(x)/-q)}{dx}$ → for e^-

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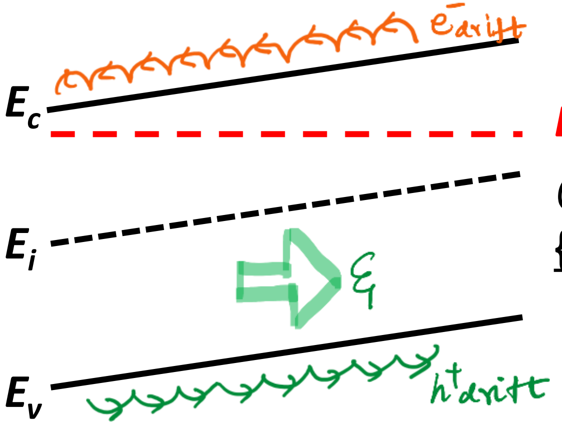

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$J_{net} = 0$

x = L

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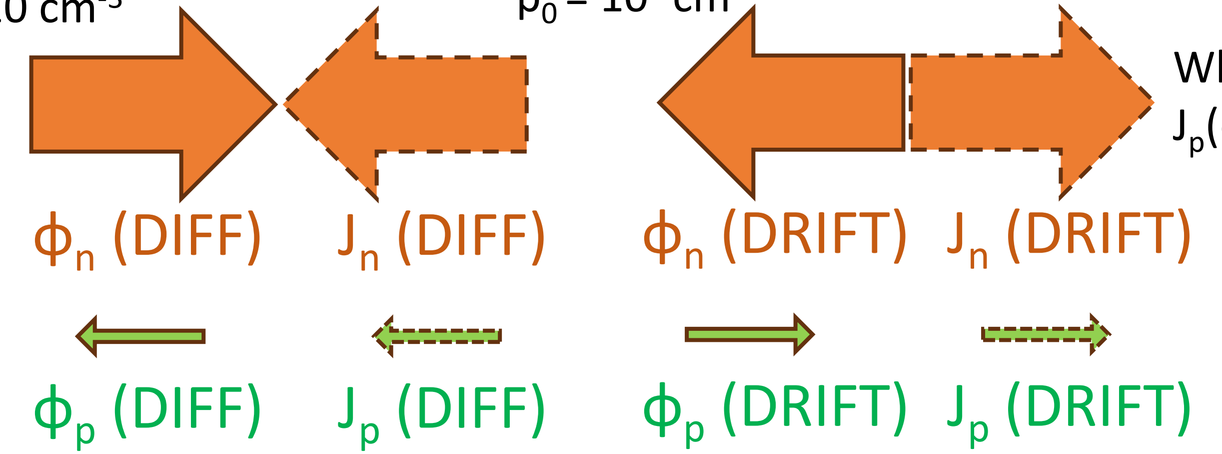

Why J_n(drift) >> J_p(drift)

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$$\mathcal{E}(x) = -\frac{dV}{dx} = \frac{-d(E_i(x)/-q)}{dx} \to \text{for } e^-$$

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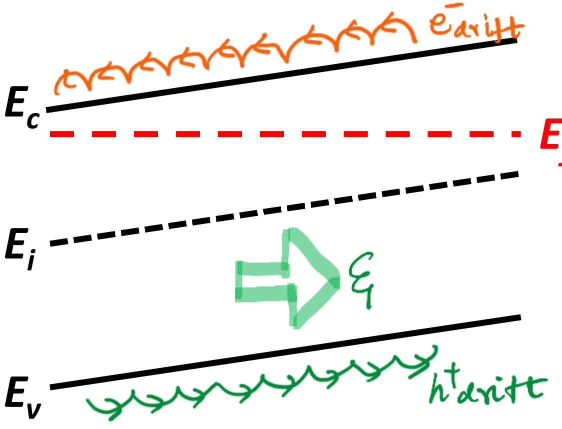
Drift Diffusion @ Thermal Equilibrium:

Example: Exponentially doped semiconductor w/o any external excitation – Band Diagram?

$$N_d(x) = N_{d0}e^{-x/\lambda}$$



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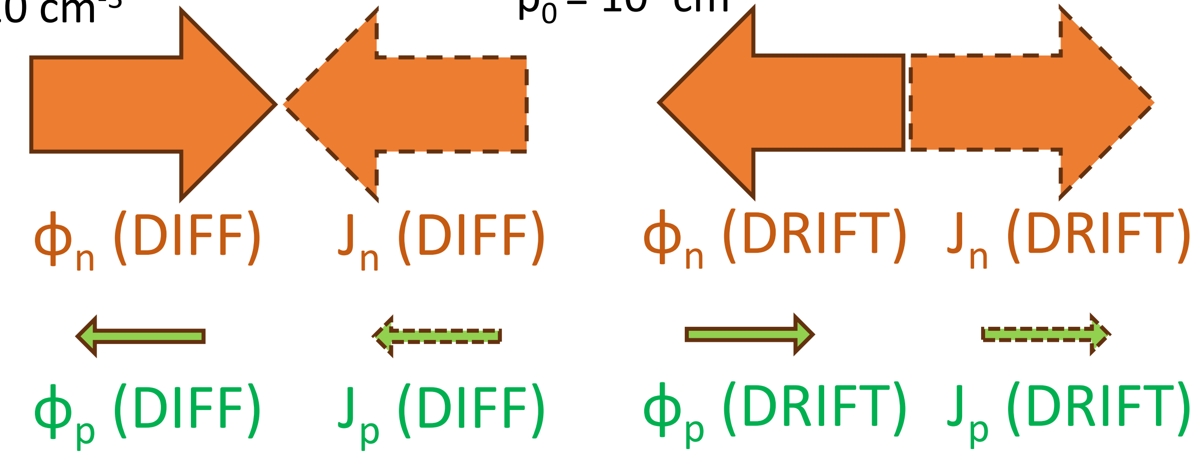

Insights !:-

Note @ Thermal Equilibrium:-

$$\left\{ \begin{array}{c} J_{net} = 0 \\ J_n = 0\,;\ J_p = 0 \end{array} \right\}$$

Individual e^- & h^+ currents drift & diff must cancel out

{Why?}

→ particle conservation!

$J_n(drift) + J_n(diff) = 0$

$J_p(drift) + J_p(diff) = 0$

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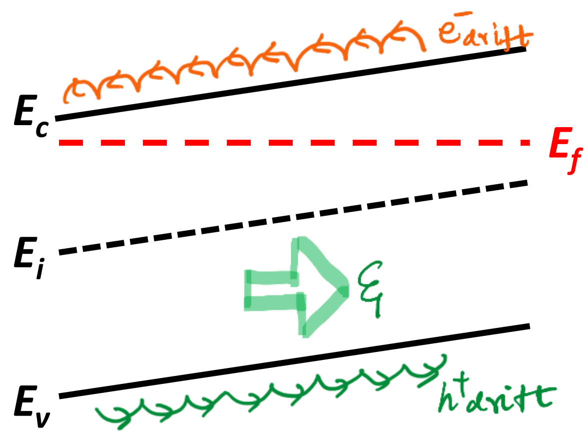
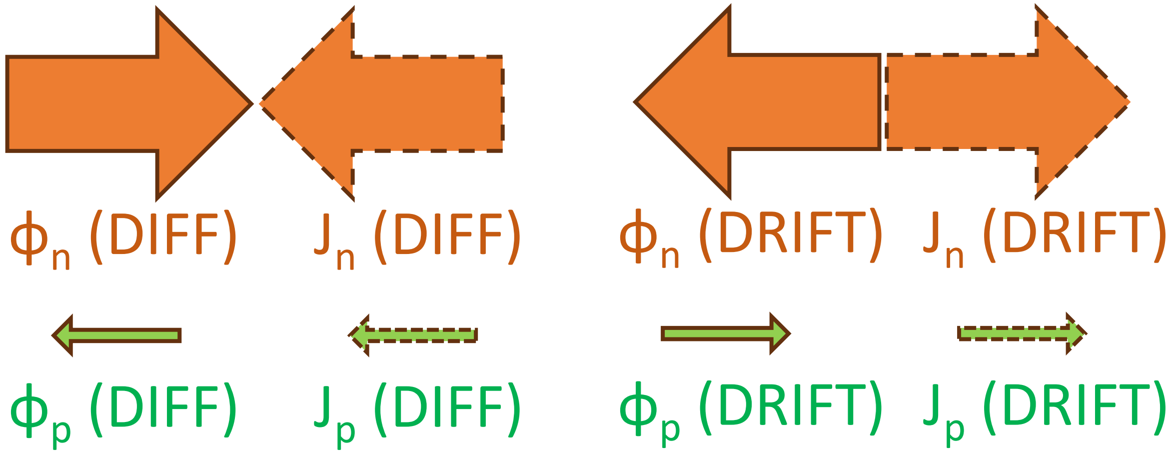
<u>Drift Diffusion @ Thermal Equilibrium:</u>

Example: Exponentially doped semiconductor w/o any external excitation – Band Diagram?

$$N_d(x) = N_{d0}e^{-x/\lambda}$$

$$J_{net} = 0$$





Insights 2:–

$$\boxed{\mathcal{E}(x) = \frac{1}{q}\frac{dE_i(x)}{dx}}$$

{ gradient in E_c, E_v indicative of $\mathcal{E}$ }

In this case,

$\mathcal{E}_{bi}$ NOT $\mathcal{E}_{ext}$

{ BUILT IN }

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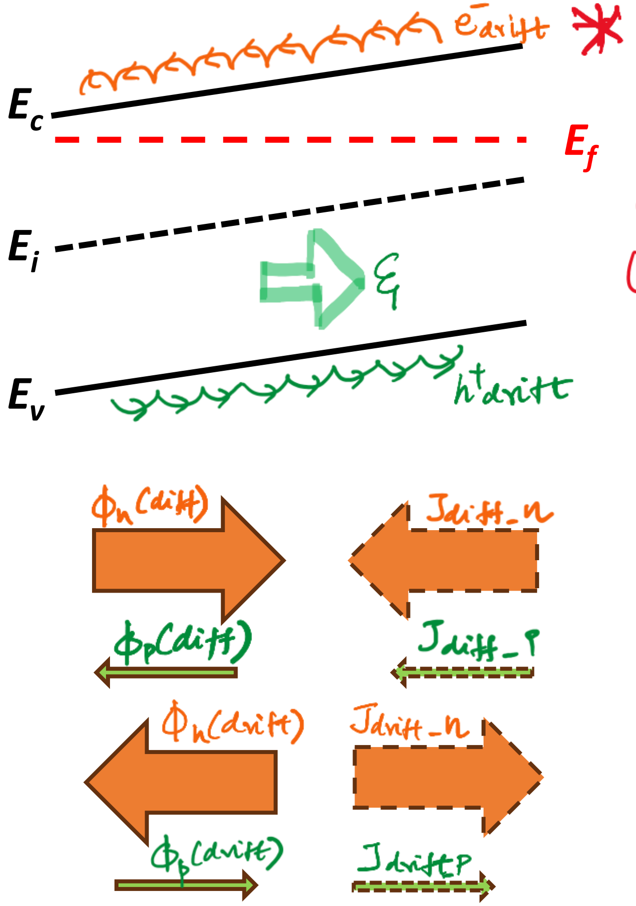
Drift Diffusion @T.E. & Einstein's relation

Exponentially doped semiconductor @ T.E.



$J_{net}=0;\ J_n=0;\ J_p=0$

{drift & diff components of e^- & h^+ cancel out

$$J_n(net)=0 \Rightarrow J_n\,diff + J_n\,drift = 0$$

$$\Rightarrow q D_n \boxed{\frac{dn(x)}{dx}} + q\mu_n n(x)\mathcal{E}(x) = 0 \quad \text{— (1)}$$

Recall

$$n(x) = n_i \exp\left[\frac{E_F(x)-E_i(x)}{k_BT}\right] \Rightarrow \frac{dn(x)}{dx} = \underbrace{n_i \exp\left[\frac{E_F(x)-E_i(x)}{k_BT}\right]}_{n(x)} \frac{1}{k_BT}\frac{d[\cancel{E_F}(x)-E_i(x)]}{dx}$$

$0\{T.E\}$

$$\frac{dn(x)}{dx} = -n(x)\frac{1}{k_BT}\frac{dE_i(x)}{dx} = -n(x)\frac{q}{k_BT}\mathcal{E}(x) \quad \text{— (2)}$$

$\sim q\mathcal{E}$

Substituting in (2) in (1)

$$-\frac{q^{\cancel{2}}}{k_BT} D_n \cancel{n(x)}\cancel{\mathcal{E}(x)} + \cancel{q}\mu_n \cancel{n(x)}\cancel{\mathcal{E}(x)} = 0$$

$$\boxed{\frac{D_n}{\mu_n} = \frac{D_p}{\mu_p} = \frac{k_BT}{q}}$$

Einstein's Relationship

Insight: True for any thermal – random motion

D and μ are intrinsically tied to carriers moving in a chaotic system undergoing collisions

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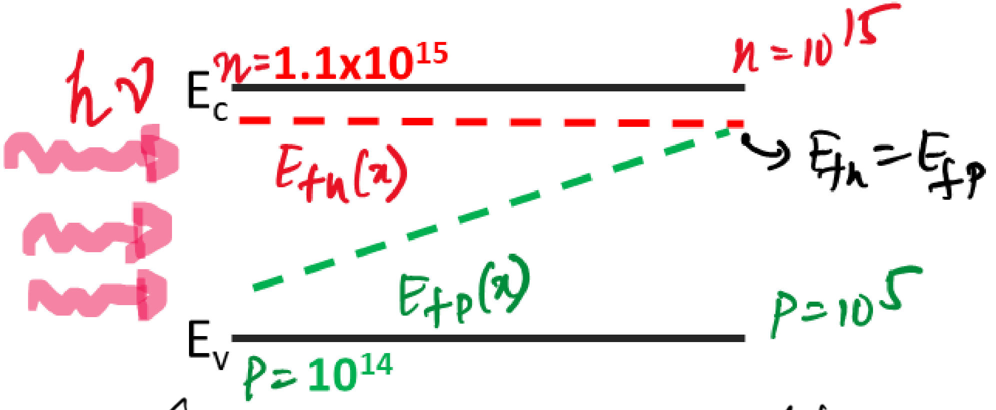
Drift Diffusion (general) Non-Thermal equilibrium (E_{fn}, E_{fp})



Same analysis as last slide!

$$J_n(x) = q D_n \boxed{\frac{d\,n(x)}{dx}} + q\mu_n n(x)\,\xi(x) \neq 0$$

$$n(x) = n_i \exp\left[\frac{E_{fn}(x) - E_i(x)}{k_B T}\right]$$

$$\boxed{\frac{d\,n(x)}{dx}} = \frac{n(x)}{k_B T}\left[\underbrace{\frac{d\,E_{fn}(x)}{dx}}_{\neq 0} - \frac{d\,E_i(x)}{dx}\right]$$

$$J_n(x) = \boxed{\frac{q D_n}{k_B T}}\, n(x)\left[\frac{d\,E_{fn}(x)}{dx} - q\,\xi(x)\right] + q\mu_n n(x)\,\xi(x)$$

$$J_n(x) = \mu_n n(x)\frac{d\,E_{fn}(x)}{dx} - \cancel{q\mu_n n(x)\,\xi(x)} + \cancel{q\mu_n n(x)\,\xi(x)}$$

$$\boxed{J_n(x) = \mu_n n(x)\frac{d\,E_{fn}(x)}{dx}\;;\; J_p(x) = \mu_p p(x)\frac{d\,E_{fp}(x)}{dx}}$$

X & ÷ by q

$$J_n(x) = \sigma_n(x)\,\frac{1}{q}\frac{d\,E_{fn}(x)}{dx}\;;\; J_p(x) = \sigma_p(x)\,\frac{1}{q}\frac{d\,E_{fp}(x)}{dx}$$

Conductance — Effective ξ for e^-; Conductance — Effective ξ for h^+

* PLEASE IGNORE THIS INTEPRETETION IF IT SEEMS CONFUSING!

Important:
- @T.E. no gradient in E_f -> $J_{net} = 0$
- @Beyond Thermal Equ: ∇E_{fn}, ∇E_{fp} -> J_n and J_p
- $J_{net} = J_n + J_p$

However, charge carriers while diffusing through semiconductor also get recombined, How to account for that? (next)

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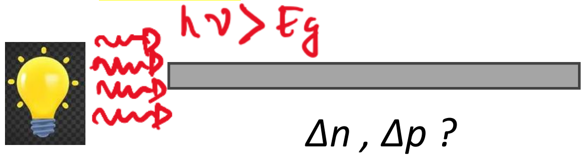
($np = n_i^2$) – Thermal Equ.

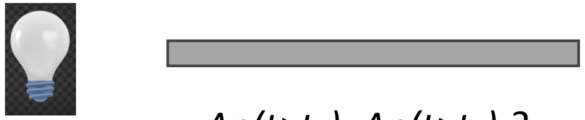
Case1: light ON at $x = 0$, t=0



$h\nu > E_g$

Δn , Δp ?
Excess carrier "Generation"

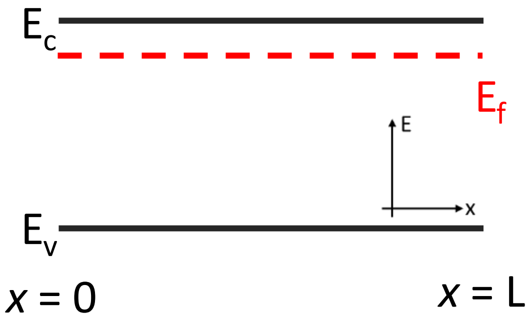
Case2: Illuminated at $x = 0$, $t = t_1$



Δn(t>t₁), Δp(t>t₁) ?
Excess carrier "Recombination"

Topic 1: Generation & Recombination

Q2) Band Diagram, E_f?



Band Diagram?

Let's consider $\Delta n = 10^{14}$ Δp=?
$\Delta p = 10^{14}$ (e-h pairs)
Now, $n = n_0 + \Delta n = 1.1 \times 10^{15}$
$p = p_0 + \Delta p \sim 10^{14}$

$np \gg n_i^2$ Position of E_f?

Fermi-level picture insufficient for non-Equilibrium!

Topic 2: Quasi-Fermi Levels

Q3) Do the Excess carriers move in the slab *Δp,n* (x)?

$J_{drift} = \sigma E$, here $E=0$
Therefore $J_{net} = 0$ No!

Spatial distribution of carriers

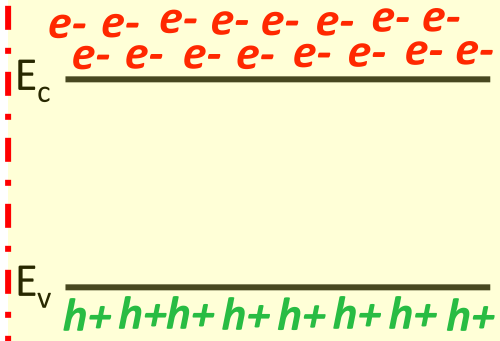
x = 0		*x = L*
$n = 10^{17}$	p- diffusion	$n = 10^{17}$
$p = 10^{15}$	$J_{p,diff}$	$p = 10^{3}$

Huge Spatial Gradient in *p* -> $\frac{dp}{dx}$

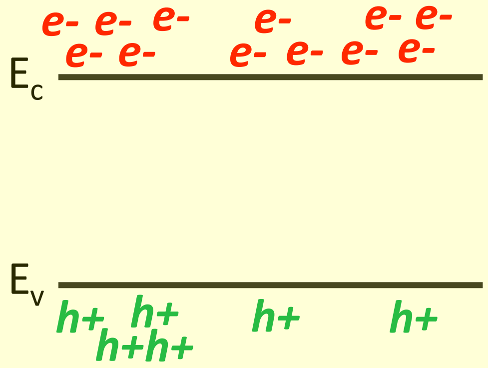
In nature: molecules diffuse from higher to lower concentration

{diffusion current}
$J_{p,diff} \propto dp/dx$

Topic 3: Drift and Diffusion



Ideal Conditions:
Only Diffusion



Real Conditions:
Diffusion + Recombination
How to account? Charge conservation

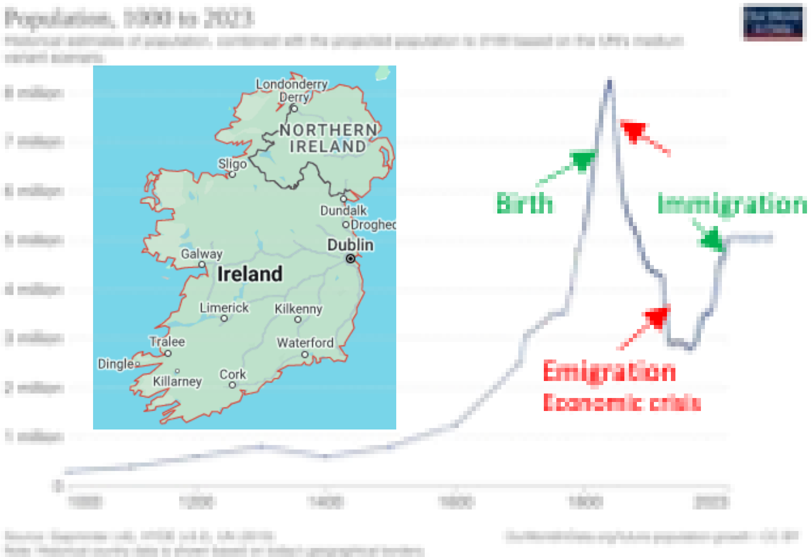
Topic 4: Carrier Continuity

Carrier Continuity – carrier book-keeping/census

Understanding carrier continuity with example: Country population census

Country Census: Population vs time

***Ireland**: interesting census*



Door to door and count people every year

OR

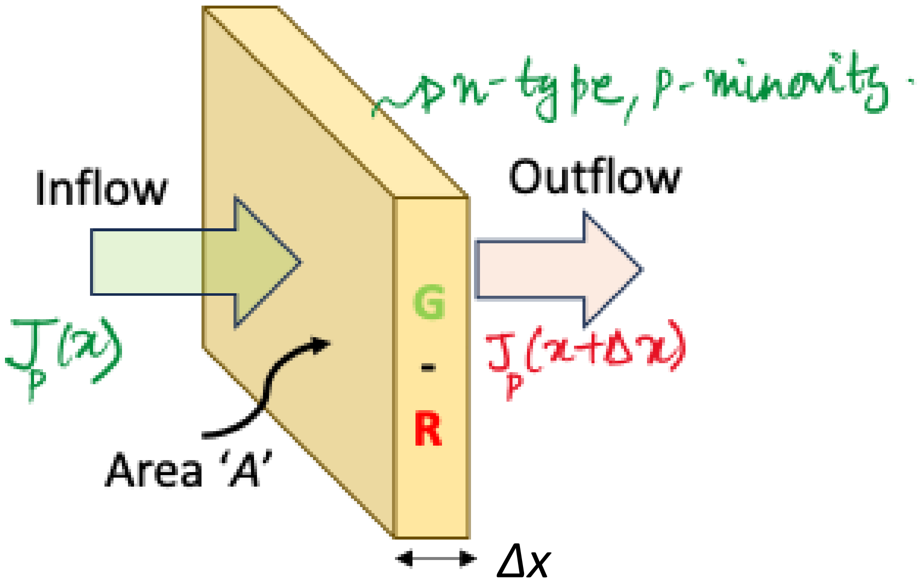
Count factors that change population

$$\frac{people}{time} = +\mathrm{R}_{\mathrm{birth}} - \mathrm{R}_{\mathrm{death}} + \mathrm{R}_{\mathrm{immigration}} - \mathrm{R}_{\mathrm{emigration}}$$

R_ = rate of _ ;
immigration: people entering;
emigration: people exiting
In essence this is just book-keeping/accounting

The same is done in case of semiconductors (country) and carrier conc. (population)!

Carrier population/conc. vs. *time*



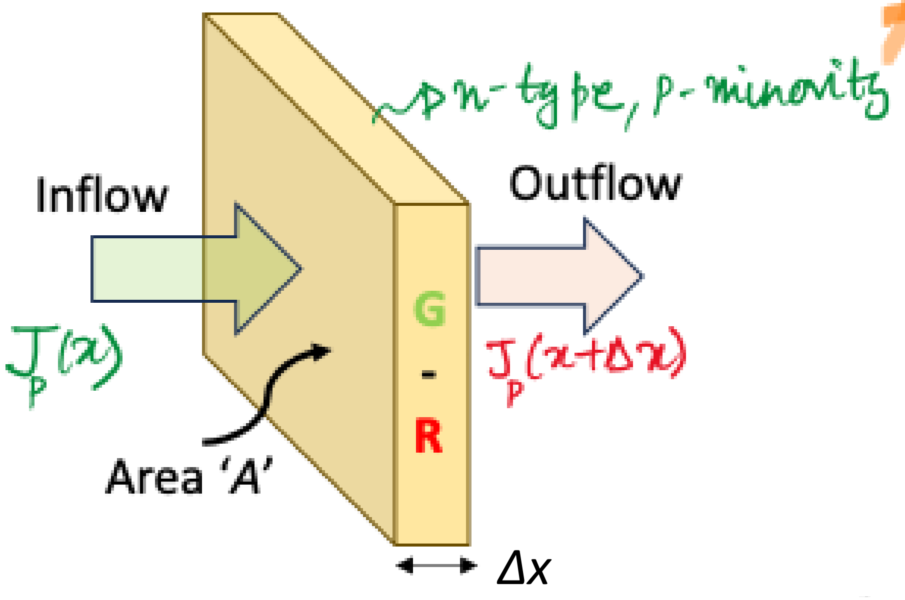
FACTORS AFFECTING $\Delta P(t)$ into Vol "$A\Delta x$"

↳ Generation, Recomb, $J(x)$, $J(x+\Delta x)$

$$\frac{dP(t)}{dt} = +G - R + \frac{dP_{in}}{dt} - \frac{dP_{out}}{dt}$$

Carrier Continuity – carrier book-keeping/census

Carrier population/conc. vs. *time*



must be related to $J_p(x)$ & $J_p(x+\Delta x)$ HOW?

$$\left(\frac{dP_{in}}{dt} - \frac{dP_{out}}{dt}\right) \times \frac{q\,\Delta x\,A}{q\,\Delta x\,A}$$

$$= \left(\frac{dQ_{in}}{dt} - \frac{dQ_{out}}{dt}\right) \times \frac{1}{q\,\Delta x\,A}$$

$$= \left[J_p(x) - J_p(x+\Delta x)\right]\frac{1}{q\,\Delta x}$$

$$= -\frac{1}{q}\,\frac{\left[J_p(x+\Delta x) - J_p(x)\right]}{\Delta x}$$

$$= -\frac{1}{q}\lim_{\Delta x \to 0}\frac{dJ_p(x)}{dx}$$

$$= -\frac{1}{q}\nabla_x J_p(x)$$

↳ Grad of J

FACTORS AFFECTING $\Delta P(t)$ into Vol 'A Δx'

↳ Generation, Recomb, $J(x)$, $J(x+\Delta x)$

$$\frac{dP(t)}{dt} = +G - R + \frac{dP_{in}}{dt} - \frac{dP_{out}}{dt}$$

$$\boxed{\begin{aligned} \frac{dP(t)}{dt} &= +G - R - \frac{1}{q}\nabla_x J_p(x) \\ \frac{dn(t)}{dt} &= G - R + \frac{1}{q}\nabla_x J_n(x) \end{aligned}}$$

Carrier Continuity Equation!

For e- and h+

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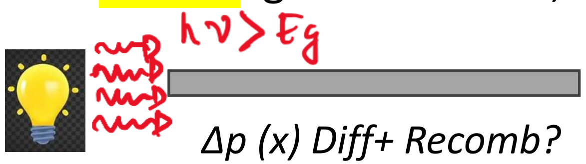
Steady state - Carrier Continuity (Recomb and Diff only)

Let's revisit our example + diode

Case1: light ON at x = 0, t=0

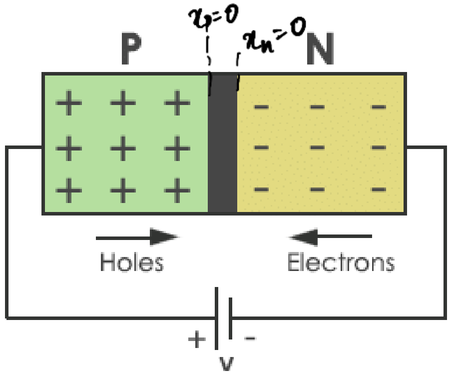
$h\nu > E_g$



Δp (x) Diff+ Recomb?

Excess carrier "Generation"

(a) optical injection



(b) electrical injection @ $x_p=0$ & $x_n=0$

In practical devices it happens often {**In Steady State**}:

- Carriers generated at one corner x = 0,
- J_{drift} negligible (Electric Field = 0)
- Minority diffusion dominant
  $(J_{rev}^{diode}, J_{sub}^{MOSFET})$
- But NET recombination everywhere due do excess carriers.

Simplifying Carrier Continuity in these cases – new insights

$$\frac{dP}{dt} = +G - R - \frac{1}{q}\frac{dJ_p(x)}{dx}$$

0 {steady-state} $\quad R_{net} \quad \frac{1}{q}\frac{dJ_{p,diff}(x)}{dx}$

$$0 = -\frac{\Delta P}{\tau_p} - \frac{1}{q}\frac{d}{dx}\left[-qD_p\frac{d\Delta P}{dx}\right]$$

$$\Rightarrow \frac{\partial^2 \Delta P}{\partial x^2} = \frac{\Delta P}{D_p \tau_p} \quad \left\{\text{Another 2nd order D.E.!}\right\}$$

$D_p \times \tau_p \rightarrow L_p^2$ {cm^2}

{diff coef $cm^2 s^{-1}$} {Recomb lifetime s} {Diffusion length}

$L_p \rightarrow$ physical meaning?

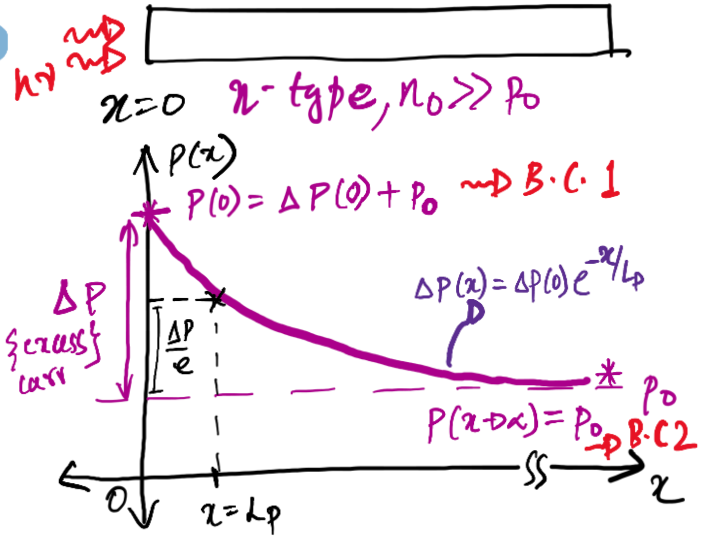
Solution:- $\Rightarrow \Delta P(x) = C_1 e^{-x/L_p} + C_2 e^{+x/L_p}$

When excess carr diffussion + recombine

#1) $\Delta P \rightarrow \Delta P/e$ @ $x = L_p$ {simple}.

#2) $x = L_p$ an average h^+ diffuses BEFORE Recombining!

* Recall Slide 6'



Furthermore, Subs $\Delta P(x)$ in J_p diff

$$J_p(diff) = -qD_p\frac{dP(x)}{dx}$$

$$= -qD_p\frac{d\,(P_0 + \Delta P(x))}{dx} = -qD_p\frac{d\Delta P(x)}{dx}$$

$$\boxed{J_p(diff) = q\frac{D_p}{L_p}\Delta P(x)}$$

$\rightarrow$ Will be used J_{diode}, BJTs etc.

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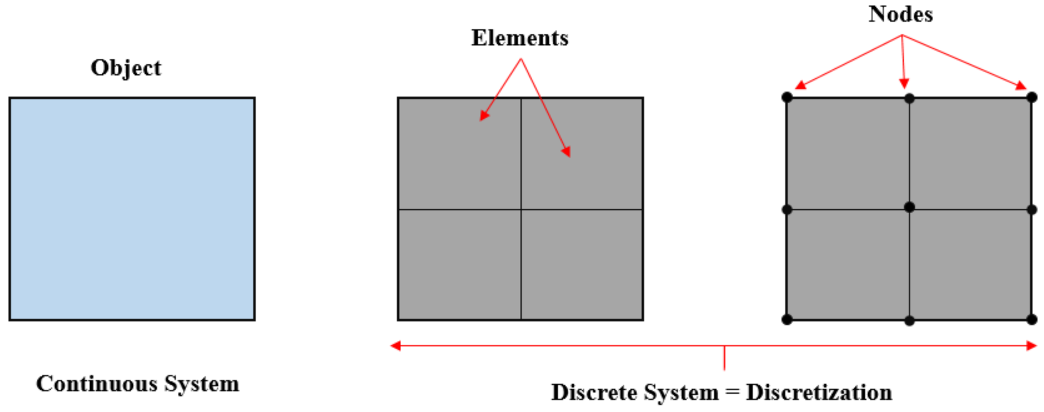
Semiconductor Device Modelling: An Overview

Now we understand the physical processes to model semiconductor devices {in semiclassical regime}

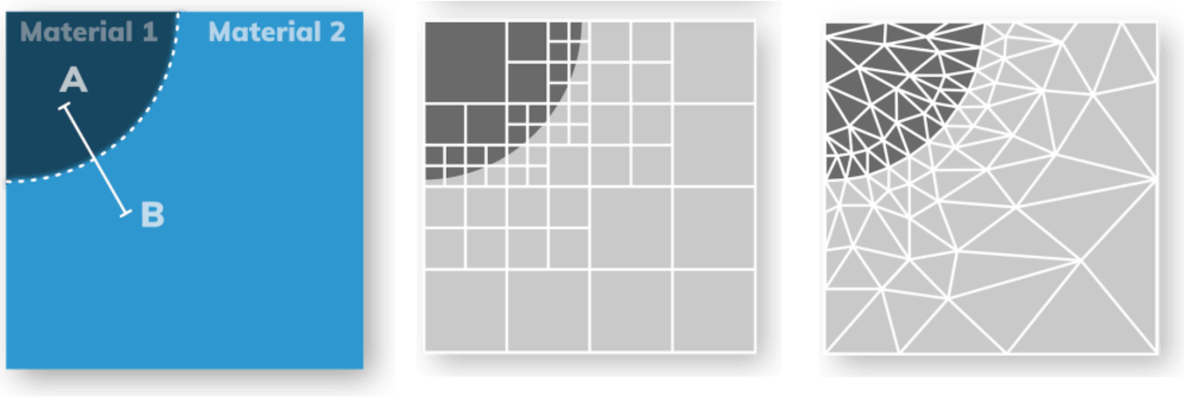
EE5181/EE2104: Only the physical phenomenon -> EE2503/EE6130: How to solve these equations on a computer?

1. Domain Discretization:

A computer cannot solve continuous domain



Equations are solved on each node

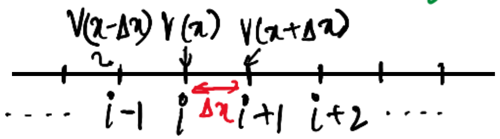


Meshing is an art, requires understanding of system
(a) domain shape (b) domain size

2. Equation Discretization:

Even the equations need to be discretized
From Differential Eqn. -> Difference Eqn.

Simple example :- $\frac{d^2V(x)}{dx^2} = 0$ } differential equation



$V(x+\Delta x)$ Taylor series expansion

$V(x+\Delta x) = V(x) + \Delta x V'(x) + \frac{(\Delta x)^2}{2!} V''(x) + O^3 \ldots$ (1)

$V(x-\Delta x) = V(x) - \Delta x V'(x) + \left(\frac{\Delta x}{2!}\right)^2 V''(x) - O^3 \ldots$ (2)

(1) + (2)

$V(x+\Delta x) + V(x-\Delta x) = 2V(x) + 2\frac{\Delta x^2}{2!} V''(x) + 2O^4 + \ldots$

Considering Δx very small, Ignoring $O^4, O^6 \ldots$

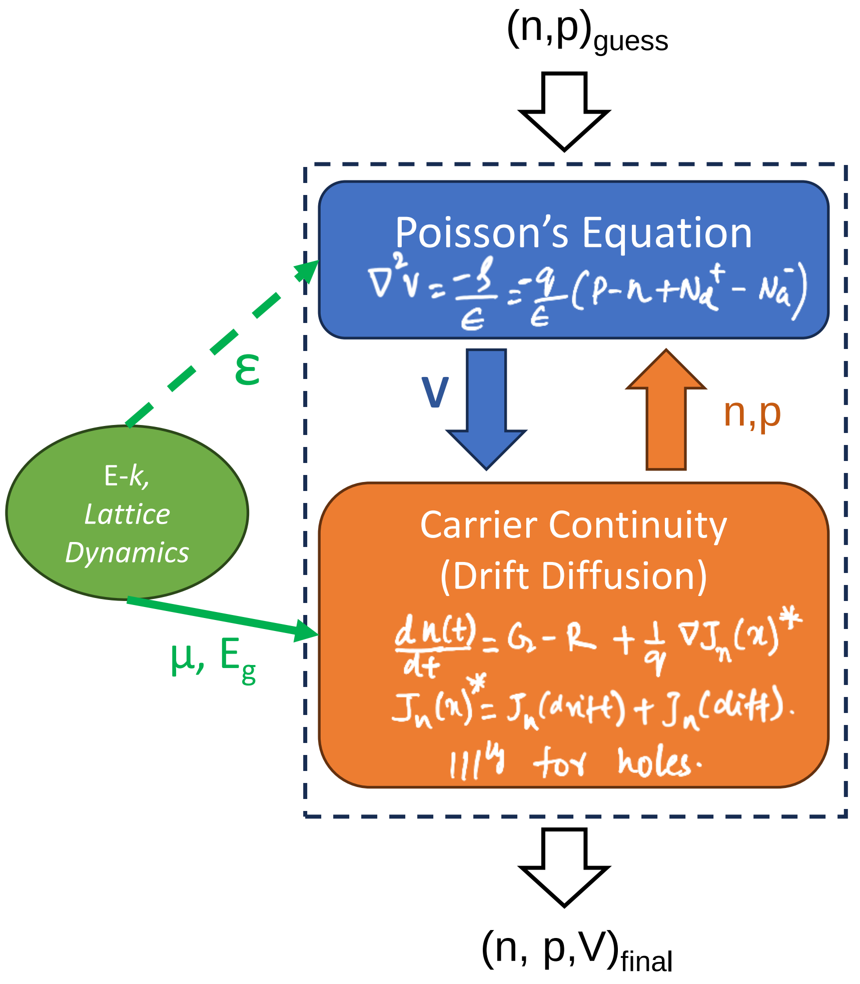
$$V''(x) \approx \frac{V(x+\Delta x) - 2V(x) + V(x-\Delta x)}{\Delta x^2}$$

$V''[i] = (V[i+1] - 2V[i] + V[i-i]) / \Delta x^2$

From Cont. Differential Eqn -> Discrete DIFFERENCE EQN.

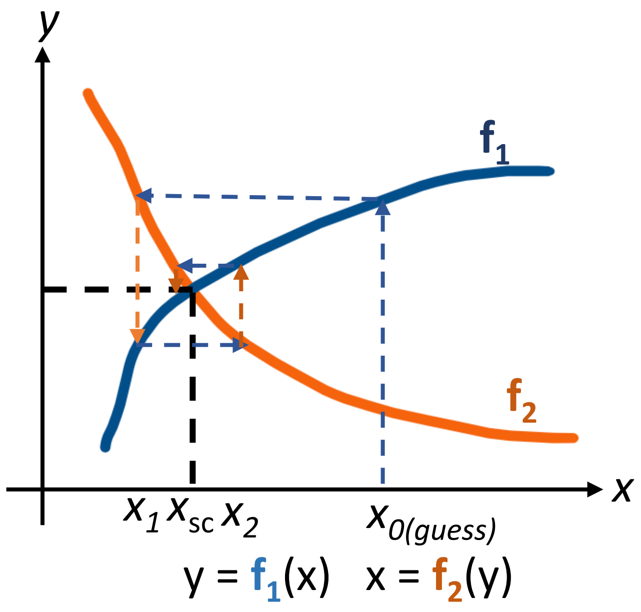
TCAD simulators: Iterative, Self-consistent solutions

TCAD simulators (Steady state)



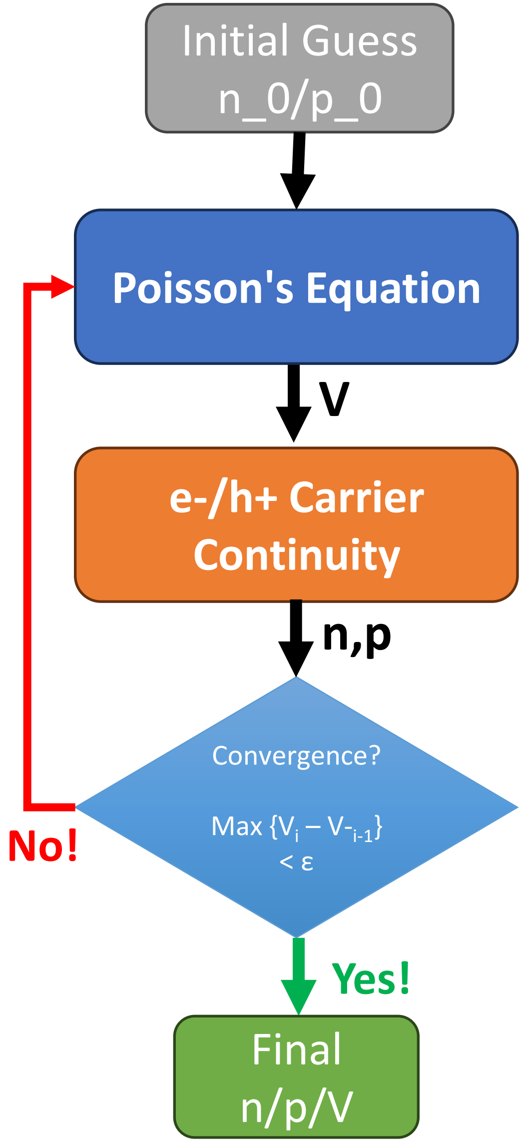
Both Equations solved
Self consistently, Iteratively

Meaning of self consistency (with an example)



Easy if f_1 and f_2 are polynomials

But here they are differential equations so bit more complicated



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Summary - Quasi Equilibrium Transport

Q: How charge carriers flow when subject to external excitation?

#1] GENERATION / RECOMBINATION :→ Steady-state {Dynamic equ} | Transient {Δn/Δp {excess}}

(IN)DIRECT & (NON) RADIATIVE. $G = R$ {Rate of gen / Recomb}

$R_{net} = -\frac{\Delta p(t)}{\tau_p}$ ⟶ $\Delta p(t) = \Delta p(0)\, e^{-t/\tau_p}$

minority recomb lifetime $\tau_p = 1/\alpha_R n_0$

#2] QUASI FERMI LEVELS :→ Thermal Equ $\{n_0 p_0 = n_i^2\}$

Single E_F → n_0, p_0 ; $\boxed{\frac{dE_F}{dx} = 0}$

BEYOND Thermal Equ. $\{np \neq n_i^2\}$ (excess carr)

$n(x) = N_c' \exp\left[\frac{E_{fn}(x) - E_c}{k_B T}\right]$

$p(x) = N_V' \exp\left[\frac{E_V - E_{fp}(x)}{k_B T}\right]$

E_{fn} ; E_{fp} } Independent F-D stats.

#3] DRIFT + DIFFUSION FORMALISM } →

$J_{n,net}(x) = \underbrace{q\mu_n n(x)\,\xi(x)}_{\text{DRIFT}} + \underbrace{qD_n \frac{dn(x)}{dx}}_{\text{DIFFUSION}}$

$J_{p,net}(x) = q\mu_p p(x)\,\xi(x) - qD_p \frac{dp(x)}{dx}$

@ Thermal Equ.

$J_n = 0 \Rightarrow J_n^{drift} = J_n^{diff}$

$J_p = 0 \Rightarrow J_p^{drift} = J_p^{diff}$

} $\frac{D_{n/p}}{\mu_{n/p}} = \frac{k_B T}{q}$

Beyond Thermal Equ

$J_n(x) = \mu_n n(x) \nabla E_{fn}$

$J_p(x) = \mu_p p(x) \nabla E_{fp}$.

#4] CARRIER CONTINUITY {Accounting / Book-keeping of carriers in Semi con.}

$\frac{dp(t)}{dt} = +G - R - \frac{1}{q}\nabla_x J_p(x)$

$\frac{dn(t)}{dt} = G - R + \frac{1}{q}\nabla_x J_n(x)$

In steady state → $\frac{dp(t)}{dt} = 0$; $R_{net} = -\frac{\Delta p(t)}{\tau_p}$, $J_p \approx J_p(\text{diff})$

$\Delta p(x) = \Delta p(x=0)\, e^{-x/L_p}$ ⇝ $J_p(\text{diff}) = q\frac{D_p}{L_p}\Delta p(x)$ [L_p → avg dist it diffuses before recomb]

#5] TCAD Simulators :- ① Domain discretisation {MESHING} | ② Diff. eqn. DISCRETISATION | ③ ELECTROSTATICS $\nabla^2 V = -\rho/\epsilon$ $\xrightarrow{V}$ CARR CONTINUITY (Drift Diff) ; CARR CONTINUITY $\xrightarrow{n,p}$ ELECTROSTATICS

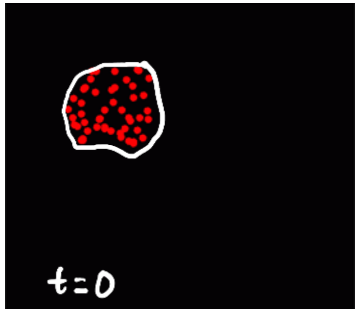
→ ITERATIVE
→ SELF-CONSISTENT

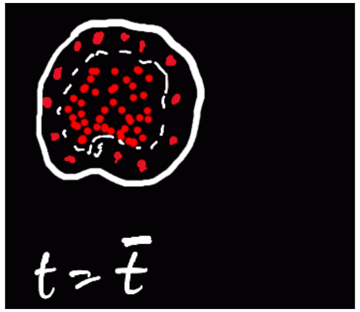
Thank you !

It was great fun taking this course for EE + ICT 2024

Please feel free to drop by my office EE507

Appendix-1: Derivation of Diffusion Current





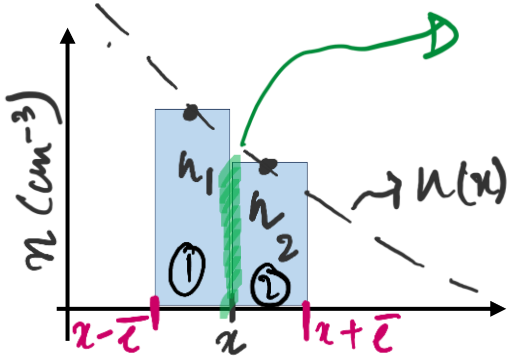
$\bar{\tau}$ {mean free time} → 't' needed for 1/2 molecules move in & out of Vol_{init}.

$\bar{l}$ {mean free path} → average dist. moved by species before random collisions

Easy to show $\phi(x) \propto \frac{d\,Conc}{dx}$ → conc.

flux → Diffusivity const?

#2 Zoom into 2 arbitrary bars & ask what is the flux through this area?



ϕ_n? → flux {no. of $\bar{e}$ per unit area per time}?

Soln:- In $\Delta t = \bar{\tau}$ {mean free path}

no. of $\bar{e}$ passing through area A = moving → +x from ① − moving ← −x from ②

$= \frac{1}{2}(n_1 \bar{l} A) - \frac{1}{2}(n_2 \bar{l} A)$

$$\phi_n \{\bar{e}/\Delta t/\Delta A\} = \frac{\bar{l}}{2\bar{\tau}}(n_1 - n_2)$$

$$\frac{n_1 - n_2}{\bar{l}} = \frac{n(x) - n(x+\Delta x)}{\Delta x}$$

$$n_1 - n_2 = \frac{[n(x) - n(x+\Delta x)]}{\Delta x}\bar{l}$$

$$= \frac{\bar{l}^2}{2\bar{\tau}} \frac{[n(x) - n(x+\Delta x)]}{\Delta x}$$

$$\phi_n(x) = \frac{\bar{l}^2}{2\bar{\tau}} \frac{-\Delta n}{\Delta x} = -\boxed{\frac{\bar{l}^2}{2\bar{\tau}}} \frac{dn(x)}{dx}$$

$\lim_{\Delta x \to 0}$

$$\boxed{\frac{\bar{l}^2}{2\bar{\tau}} = D_n}$$

→ Coeff of diffusion

$$\phi_n(x) = -D_n \frac{dn(x)}{dx}$$

−ve?

$$J_{n,diff} = (-q)(-D_n)\frac{dn(x)}{dx}$$

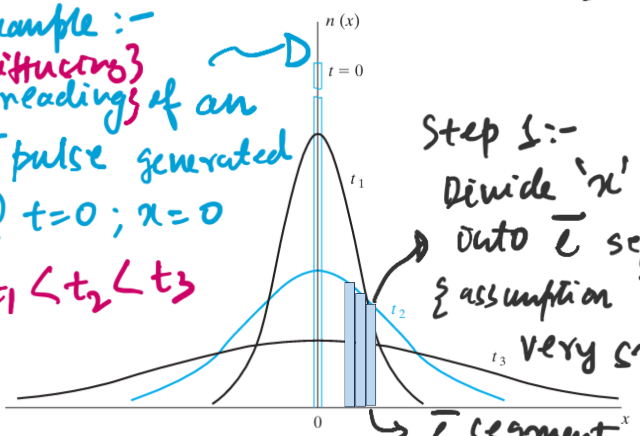
$$\boxed{J_{n,diff} = qD_n \frac{dn(x)}{dx}}$$

$$\boxed{J_{p,diff} = -qD_p \frac{dp(x)}{dx}}$$

$\bar{e}$ & h^+ diff curr.

example :- {diffusion} → {spreading} of an $\bar{e}$ pulse generated @ t=0 ; x=0

$t_1 < t_2 < t_3$



Step 1:- Divide 'x' axis into $\bar{l}$ segments {assumption $\bar{l}$ is very small}

→ $\bar{l}$ segment.