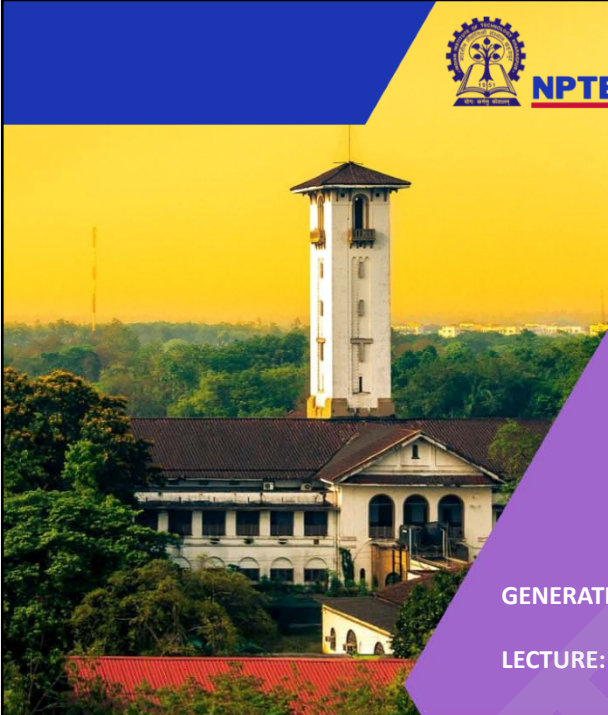





NPTEL ONLINE CERTIFICATION COURSE


**SEMICONDUCTOR DEVICE
MODELING AND SIMULATION**

PROF. VIVEK DIXIT
 Department of Electronics and Electrical Communication
 Engineering
 Indian Institute of Technology Kharagpur

GENERATION-RECOMBINATION

 LECTURE: 44


L44 GENERATION AND RECOMBINATION


- Generation-Recombination mechanisms

$$\frac{dn}{dt} = \frac{1}{q} \frac{dJ_n}{dx} + G - \frac{\delta n}{\tau}$$

$$\frac{dp}{dt} = -\frac{1}{q} \frac{dJ_p}{dx} + G - \frac{\delta p}{\tau}$$

$G = -R$
 $-R \approx \frac{\delta n}{\tau}$ ← excess carrier conc.

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



GENERATION-RECOMBINATION (GR)



- At equilibrium charge distributions: $np = n_i^2$ *low no. max. return*
- When the system is perturbed, the system tries to restore itself towards equilibrium through recombination-generation
- Steady-state recombination rate will be proportional to the deviation from equilibrium,
 - $R \propto (np - n_i^2)$ *recomb $\propto np$*

$$= k np = \frac{k n_i^2}{\tau_{gen}}$$

$$R = (r_{com} - g_{en}) = k (np - n_i^2)$$

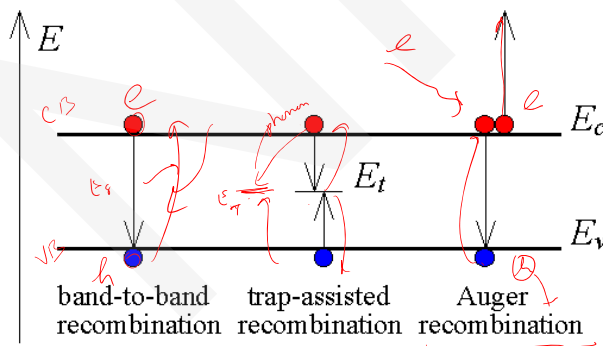
SEMICONDUCTOR DEVICE MODELING AND SIMULATION



GR MECHANISMS

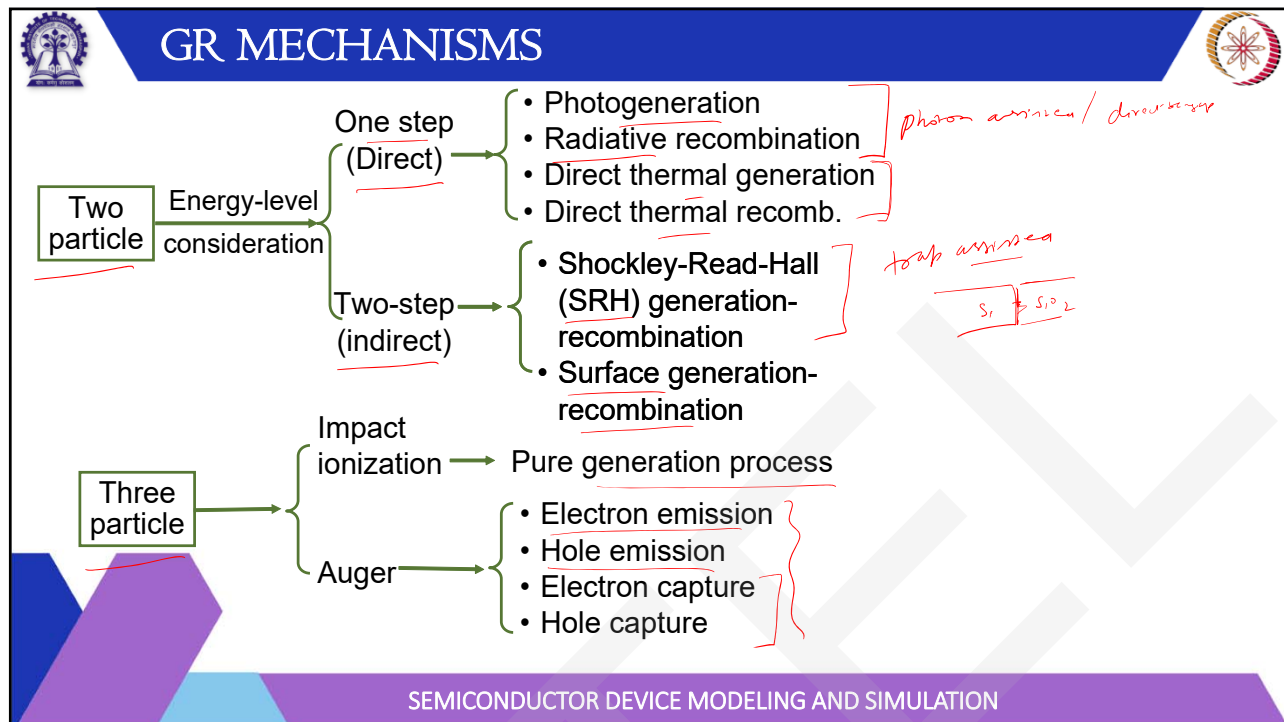


- Recombination: process by which electrons and holes annihilate each other i.e. : electrons occupy - through one or multiple steps - the empty state associated with a hole.
- Energy released as- photon / phonon / kinetic energy of a carrier



- These recombination mechanisms are reversible, i.e., carrier generation.
- A single expression can be used to describe generation-recombination

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



GR MECHANISMS

1. Band-to-Band Recombination, i.e. direct thermal recombination, involves the electron falling from an allowed conduction band state into a vacant valence band state. This process is typically radiative. Eg Lasers, LEDs

Energy space

Real space

$$R = \alpha_r (np - n_i^2) = \frac{\delta n}{\tau}$$

$$\begin{aligned} n &\rightarrow n_0 + \delta n \\ p &\rightarrow p_0 + \delta p \end{aligned}$$

$$R = \alpha_r ((n_0 + \delta n)(p_0 + \delta p) - n_i^2)$$

$$= \alpha_r (n_0 p_0 + n_0 \delta p + p_0 \delta n - n_i^2)$$

$$R = \alpha_r (n_0 \delta p + p_0 \delta n)$$

2 here - velocity

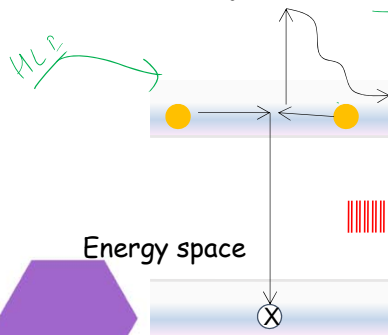
SEMICONDUCTOR DEVICE MODELING AND SIMULATION



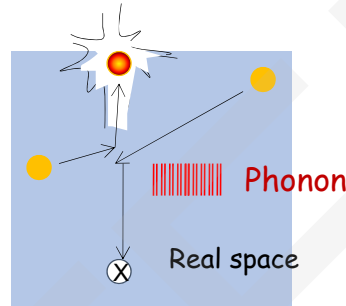
GR MECHANISMS



3. Auger Recombination: a non-radiative process, where band-to-band recombination or trapping at a band gap center occurs simultaneously with the collision between two like carriers. The surviving carrier takes away the energy and thermally loses it. Dominates in highly doped III-Vs, concentrator type solar cells, junction lasers, and LEDs.



$$C_n, C_p \sim 10^{-30} \text{ cm}^6 / \text{s at } 300\text{K}$$



$$R = (np - n_i^2)(nC_n + pC_p)$$

$$\begin{aligned} n &= n_0 + \delta n, \quad p = p_0 + \delta p \\ R &= (n_0 \delta p + p_0 \delta n + \delta n \delta p) \\ &= (n_0 + \delta n) C_n + (p_0 + \delta p) C_p \\ n_0 \ll \delta n \approx p &\ll p_0 = N_A \\ R &= p_0 \delta n C_p = \frac{p_0^2 C_p \delta n}{\tau} \\ &= \frac{\delta n^3}{C_p} \end{aligned}$$

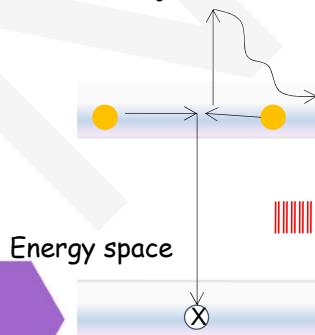
SEMICONDUCTOR DEVICE MODELING AND SIMULATION



GR MECHANISMS



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$$C_n, C_p \sim 10^{-30} \text{ cm}^6 / \text{s at } 300\text{K}$$

$$R = (np - n_i^2)(nC_n + pC_p)$$

$$LLI - n_0 \ll \Delta n = \Delta p \ll p_0 = N_A$$

$$\frac{1}{\tau} = C_n N_A^2$$

$$HLI - \delta = \Delta n = \Delta p \gg p_0, n_0$$

$$\frac{1}{\tau} = (C_n + C_p) \delta^2$$

$$\begin{aligned} R &= \delta n p_0 (\delta n C_p + p_0 C_p) \\ &= \delta n^3 C_p \\ &= \frac{\delta n^3}{C_p} \end{aligned}$$

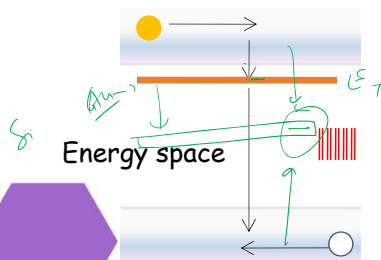
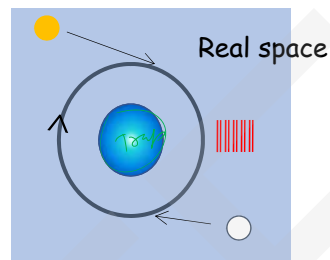
SEMICONDUCTOR DEVICE MODELING AND SIMULATION



GR MECHANISMS



4. R-G Center (indirect thermal) Recombination: R-G centers, energy levels (E_T) introduced by certain impurity atoms or crystal defects into the midgap region of a semiconductor, act as intermediaries in the recombination process. The capture of an electron and a hole at the same site leads to the annihilation of the electron-hole pair. This process is characteristically non-radiative.



$$R = \frac{np - n_i^2}{\tau_p(n + n_i) + \tau_n(p + p_i)}$$

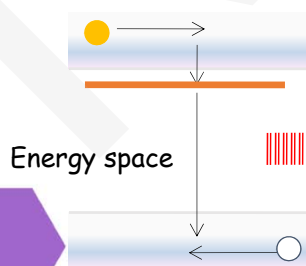
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GR MECHANISMS



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$$LLI - n_0 \ll \Delta n = \Delta p \ll p_0 = N_A$$

$$\tau = \tau_n$$

$$HLI - \delta = \Delta n = \Delta p \gg p_0, n_0$$

$$\tau = \tau_n + \tau_p$$

$$\text{Depletion} - n \sim p \sim 0$$

$$R = \frac{-n_i^2}{\tau_p(n_i) + \tau_n(p_i)}$$

$$R = \frac{np - n_i^2}{\tau_p(n + n_i) + \tau_n(p + p_i)}$$

$$\begin{aligned} \frac{\beta_i \delta n}{\tau_n p_0} &= \frac{\delta n}{\tau} \\ &= \frac{\delta n \delta p}{\tau_p \delta n + \tau_n \delta p} = \frac{\delta}{\tau_p n_i + \tau_n p_i} \\ &= -\frac{n_i^2}{\tau_p n_i + \tau_n p_i} \end{aligned}$$

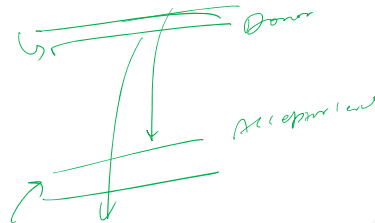
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GR MECHANISMS



5. Recombination via Shallow Levels: Donor and acceptor sites function R-G centers, extremely inefficient at room temperature, in the recombination process. The largest energy step is typically radiative.



SEMICONDUCTOR DEVICE MODELING AND SIMULATION

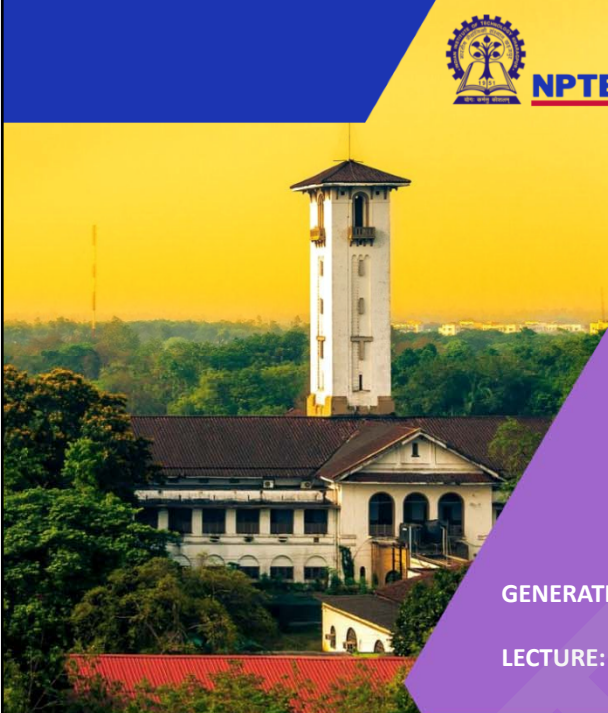


CONCLUSION



- Discussed various recombination processes

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GENERATION-RECOMBINATION

 LECTURE: 45



L45 GENERATION AND RECOMBINATION



- *Generation-Recombination mechanisms - derivation and measurements*

$$\frac{dn}{dt} = \frac{1}{q} \frac{dJ_n}{dx} + G - \frac{\delta n}{\tau}$$

$$\frac{dp}{dt} = -\frac{1}{q} \frac{dJ_p}{dx} + G - \frac{\delta p}{\tau}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



LUMINESCENCE



Luminescence - ^{cold} process of emitting light When electron-hole pairs are generated or carriers are excited into higher energy levels from which they fall to their equilibrium states.

➤ **Photoluminescence** - carriers excited by photon absorption

- **fluorescence** - fast luminescent processes (10^{-8} sec)
- **phosphorescence** - slow (second or minutes) luminescent processes.

bulb - incandescence hot

*← hν
phosphorescence
→ trap*

➤ **Cathodoluminescence** - carriers created by high-energy electron bombardment

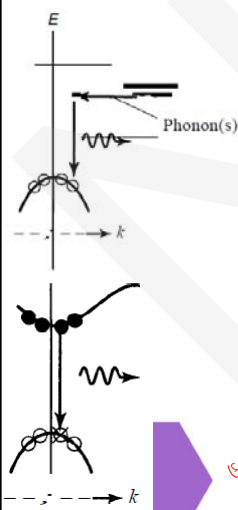
➤ **Electroluminescence** - excitation occurs by electric current (eg LED)



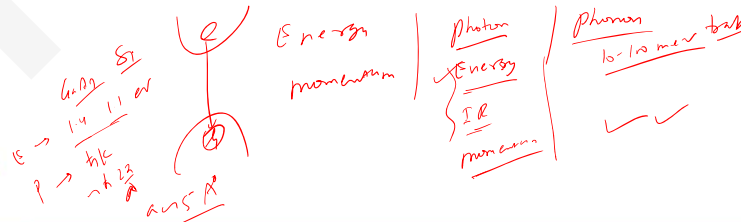
SEMICONDUCTOR DEVICE MODELING AND SIMULATION



PROPERTIES OF GR PROCESS



- crystal momentum and energy is conserved
- Band-to-band recombination is much faster in direct gap semiconductors
- R-G center process is important in indirect gap semiconductors
- Usually only dominant process matters
- band-to-band or R-G center recombination-generation usually dominant in low-field regions of a non-degenerately doped semiconductor maintained at room temperature.



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MOMENTUM CONSIDERATION

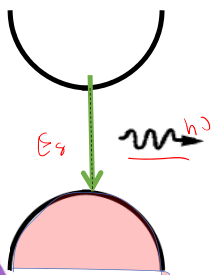
Conserve Energy $E_g = h\nu$

Conserve momentum $\Delta k = k_{\text{photon}} = \frac{2\pi\nu}{c} = E_g/\hbar c$

$\Delta k \sim 6/\mu\text{m}$ ($E_g \sim 1.2 \text{ eV}$) $\ll$ $BZ = 2\pi/a \sim 1/\text{\AA}$ for $a=5.43 \text{ \AA}$ Optical transitions almost vertical !!

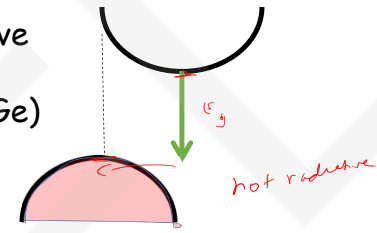
$\frac{1}{10^{-10} \text{ m}} \gg$

Direct bandgap



photons making vertical transitions won't conserve momentum for indirect band-gaps (Si, Ge)

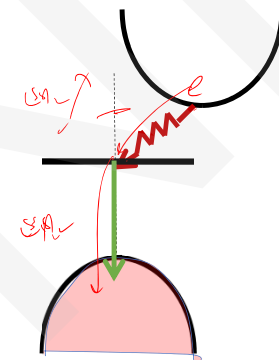
Indirect bandgap



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MOMENTUM CONSIDERATION

Indirect Band-gap



Conserve momentum ✓

$$\Delta k = k_{\text{phonon}} = \frac{2\pi\nu_{\text{phonon}}}{v_{\text{sound}}} = E_{\text{phonon}}/\hbar v_{\text{sound}} \approx \frac{2\pi}{a} [\text{\AA}]$$

Atomic displacements are involved, Wavelengths are Comparable

Conserve Energy

$$E_{\text{phonon}} = \hbar\nu_{\text{phonon}} \sim 10\text{-}100 \text{ meV} \ll E_g$$

Two step process !!

$k_{\text{trap}} \approx \frac{2\pi}{a}$

E_g for Si,
 $v_L = 8430 \text{ m/s}$ along [100]
 $\nu_{\text{LTO}}(\Gamma_{25'}) = 15.5 \times 10^{12} \text{ Hz}$ $T=300\text{K}$
<http://www.ioffe.ru/SVA/NSM/Semicond/Si/mechanic.html>

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



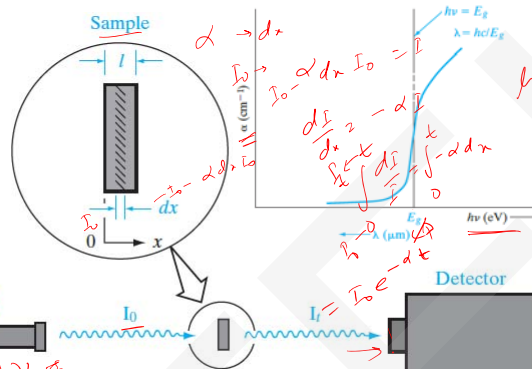
OPTICAL ABSORPTION



- Relative transmission of the photons is observed. *Used to measure band gap energy*
- I_0 = photon beam of intensity (photons/cm²-s)
- λ = photons of wavelength, selected by a monochromator
- l = sample of thickness, α =absorption coefficient (cm⁻¹)

$$\frac{dI}{dx} = -\alpha I$$

Beam intensity at a distance x from the surface, $I(x) = I_0 e^{-\alpha x}$



SEMICONDUCTOR DEVICE MODELING AND SIMULATION



PHOTOCONDUCTIVITY



- Excess electrons and holes creation → conductivity increases
- **photoconductivity** - if excess carriers due to optical luminescence
- every semiconductor device depends in some way on the recombination of excess electrons and holes

Let us examine mechanisms by which excess electrons and holes recombine

$$\begin{aligned} G &= n e \mu_n + p e \mu_p \\ &= (n_0 + \delta n) e \mu_n + (p_0 + \delta p) e \mu_p \end{aligned}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



DIRECT RECOMBINATION



- Excess electrons and holes decay by electrons falling from CB to empty states (holes) in VB. (photon emission)
- Spontaneous process i.e. constant probability that an electron and a hole will recombine, α_r
- rate of decay of electrons at any time t ,

$$\frac{dn(t)}{dt} = \underbrace{\alpha_r n_i^2}_{\text{Thermal generation}} - \underbrace{\alpha_r n(t)p(t)}_{\text{Recombination}}$$

- $\delta n(t), \delta p(t)$ = instantaneous excess carrier concentrations

$$\begin{aligned} \frac{d\delta n(t)}{dt} &= \alpha_r n_i^2 - \alpha_r [n_0 + \delta n(t)][p_0 + \delta p(t)] \\ &= -\alpha_r [(n_0 + p_0)\delta n(t) + \delta n^2(t)] \end{aligned}$$

$\delta n = \delta p$

$$\alpha_r n p = \alpha_r n_i^2$$

$$\frac{r}{r - \delta} = \frac{\alpha_r (n_0 + \delta n)(p_0 + \delta p)}{\alpha_r n_i^2}$$

$$n = \frac{n_0 + \delta n}{p_0 + \delta p}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



DIRECT RECOMBINATION



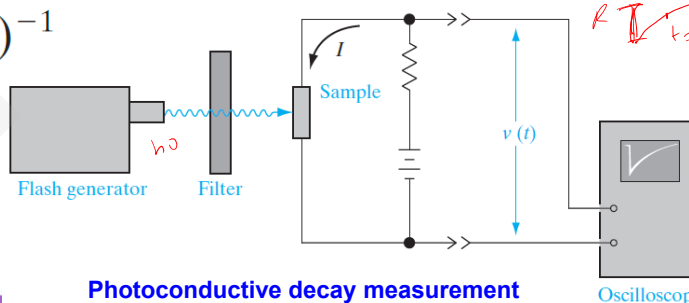
- Case: Low level injection ($\delta n(t=0) \ll p_0$ for p-type)

- Equation simplifies to $\frac{d\delta n(t)}{dt} = -\alpha_r p_0 \delta n(t)$

- Solution, $\delta n(t) = \Delta n e^{-\alpha_r p_0 t} = \Delta n e^{-t/\tau_n}$

- Minority carrier lifetime,

$$\tau_n = (\alpha_r p_0)^{-1}$$



Photoconductive decay measurement

Oscilloscope

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



QUASI FERMI-LEVEL



➤ At thermal equilibrium $g(T) = \alpha_r n_i^2 = \alpha_r n_0 p_0$

➤ Light turned on (optical generation)

$$g(T) + g_{op} = \alpha_r np = \alpha_r (n_0 + \delta n)(p_0 + \delta p)$$

➤ For low level excitation, $g_{op} = \alpha_r (n_0 + p_0) \delta n = \frac{\delta n}{\tau_n}$

➤ Excess carriers, $\delta n = \delta p = g_{op} \tau_n$

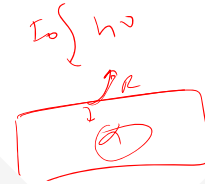
$$\delta n = \tau_n g_{op} \quad \text{and} \quad \delta p = \tau_p g_{op} \quad \text{general expression (with trapping)}$$

➤ Calc E_{fn}, E_{fp}

$$n = n_i e^{(F_n - E_i)/kT} \quad \text{and} \quad p = n_i e^{(E_i - F_p)/kT}$$

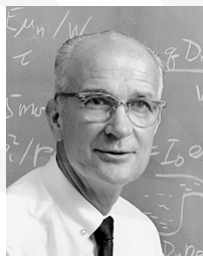
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$$g_{op} = \frac{I_0 (1-R) \alpha e^{-\alpha x}}{(hc/\lambda_{ph})}$$

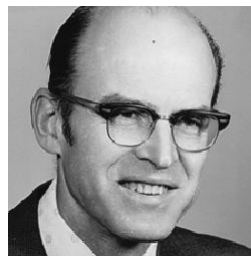


$$I_0 (1-R) \alpha e^{-\alpha x}$$

INDIRECT RECOMBINATION



William Shockley



Robert N. Hall

Also called
Shockley-Read-Hall (SRH) Recombination

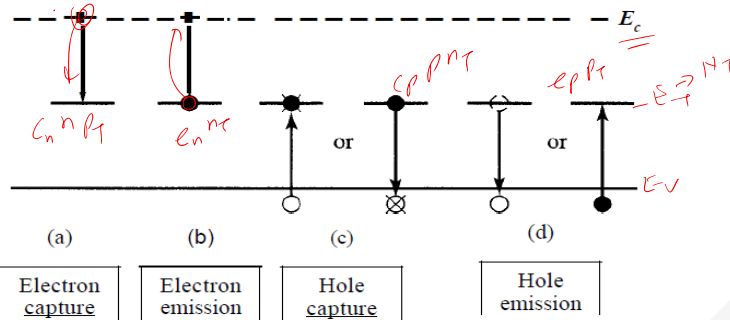
SEMICONDUCTOR DEVICE MODELING AND SIMULATION



GR STATISTICS



Electronic transitions between a single-level R-G center and energy bands



$$\left. \frac{\partial n}{\partial t} \right|_{R-G} = \left. \frac{\partial n}{\partial t} \right|_{(a)} + \left. \frac{\partial n}{\partial t} \right|_{(b)}$$

$$\left. \frac{\partial p}{\partial t} \right|_{R-G} = \left. \frac{\partial p}{\partial t} \right|_{(c)} + \left. \frac{\partial p}{\partial t} \right|_{(d)}$$

$$r_N = -\frac{\partial n}{\partial t} = c_n n p_T - e_n n_T$$

$$r_P = -\frac{\partial p}{\partial t} = c_p p_T - e_p p_T$$

- n_T = number of filled (with electron) R-G centers cm^{-3}
- p_T = number of empty R-G centers cm^{-3}
- N_T = Total number of R-G centers cm^{-3}
- c_n = the electron capture coefficient (cm^3/sec)
- e_n = the electron emission coefficient (1/sec)

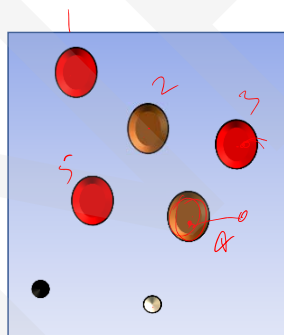
$$c_n n p_T = e_n n_T$$

$$c_n = e_n \left(\frac{n_T}{n p_T} \right)$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



CAPTURE PROCESS



$$N_T = n_T + p_T$$

$$5 = 3 + 2$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



CAPTURE RATE



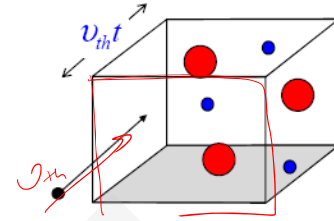
$dn/dt = \# \text{ of electron in small volume} \times \text{relative cross section of empty traps} / \text{time}$

Thermal velocity, $v_{th} = \sqrt{3kT/m^*} \sim 10^7 \frac{\text{cm}}{\text{s}}$ at 300 K

Volume = $A v_{th} t$,

fractional area for capture = $p_T A \sigma_n v_{th} t / A$

prob of capture/sec = $p_T \sigma_n v_{th} = c_n p_T$



$$\frac{dn}{dt} = -n \times \left[\frac{A \times v_{th} t \times p_T \times \sigma_n}{A \times t} \right] = -n v_{th} p_T \sigma_n$$

$$\equiv -c_n p_T n \quad c_n \equiv \sigma_n v_{th}$$

Assumption: these c's don't change under bias

$$n \times \frac{A v_{th} t \times p_T \times \sigma_n}{A t}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



GR STATISTICS



Under equilibrium:

- self balancing of each fundamental process
- $r_N = 0$ and $r_P = 0$

$$e_{n0} = c_{n0} p_{T0} n_0 / n_{T0} = c_{n0} n_1$$

$$e_{p0} = c_{p0} n_{T0} p_0 / p_{T0} = c_{p0} p_1$$

- Assuming emission and capture coefficient remain approximately equal to their equilibrium value

$$e_n \approx e_{n0} = c_{n0} n_1 \approx c_n n_1$$

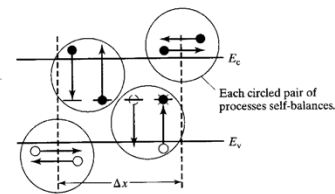
$$e_p \approx e_{p0} = c_{p0} p_1 \approx c_p p_1$$

$$n_0 = n_i \exp((E_F - E_i)/kT)$$

- For nondegenerate semiconductor

$$n_{T0}/N_T = 1/(1 + \exp((E_T' - E_F)/kT), E_T' = E_T + kT \ln g_T \text{ and } g_T \text{ is degeneracy factor}$$

$$n_1 = n_i \exp((E_T' - E_i)/kT) \text{ and } p_1 = n_i \exp((E_i - E_T')/kT)$$



$$r_N = -\frac{\partial n}{\partial t} = c_n (np_T - n_1 n_T)$$

$$r_P = -\frac{\partial p}{\partial t} = c_p (pn_T - p_1 p_T)$$

$$r_n = r_p = 0$$

$$n_1 = \frac{p_T n_0}{n_T}$$

$$= \frac{p_T n_0}{n_T} \frac{1 + \exp((E_T' - E_F)/kT)}{1 + \exp((E_T' - E_F)/kT)}$$

$$= n_0 \left(\frac{1 + \exp((E_T' - E_F)/kT)}{1 + \exp((E_T' - E_F)/kT)} \right)$$

$$= n_0 \left(\exp\left(\frac{E_T' - E_F}{kT}\right) \right)$$

$$n_0 = n_i \exp\left(\frac{E_F - E_i}{kT}\right) = n_i \exp\left(\frac{E_T' - E_i}{kT}\right)$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



GR STATISTICS



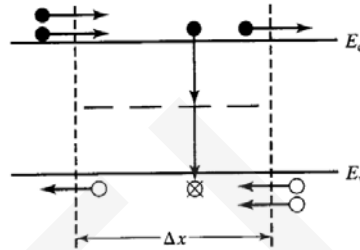
- **Under steady state:** status quo is maintained by trade-off b/w processes
(Assume emission and capture coefficient $\approx$ equilibrium value)

• $r_N = r_P$

• $n_T = \frac{c_n N_T n + c_p N_T p_1}{c_n(n+n_1) + c_p(p+p_1)}$

• $R \equiv r_N \equiv r_P = \frac{np - n_i^2}{\tau_p(n+n_1) + \tau_n(p+p_1)}$

• $\tau_p = \frac{1}{c_p N_T}$ and $\tau_n = \frac{1}{c_n N_T}$ are hole and electron minority carrier lifetimes



$\downarrow$ $n_0 + p_0 \leq p_{0, \text{max}}$

$R = \frac{n_s p_s - n_i^2}{\tau_p(n_s + n_1) + \tau_n(p_s + p_1)}$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



GR STATISTICS – TYPICAL VALUES



	N_T	E_T	σ_N	σ_P	S_N	S_P
Material	[cm ⁻³]	[eV]	[m ²]	[m ²]	[m/s]	[m/s]
Si, Ge	<u>1e13</u>	<u>0.0</u>	<u>1e-15</u>	<u>1e-15</u>	<u>0.0</u>	<u>0.0</u>
III-Vs	<u>2e16</u>	<u>0.4</u>	<u>1e-14</u>	<u>1e-13</u>	<u>0.0</u>	<u>0.0</u>

$\rightarrow$ surface

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



MINORITY CARRIER LIFETIME



- The R-G centers are typically impurities that were unintentionally incorporated into the lattice during growth or processing
- Lifetime is decreased by adding impurities (Au to Si)
- Lifetime is increased by gettering impurities
 - diffuse phosphorous into the back side of an Si device in order to trap impurities and increase the lifetimes

Table 5.1 Observed Carrier Lifetimes in Si (300 °K).

Lifetime Range	Result-Reference	Device Structure
10^{-4} – 10^{-2} sec	$\tau_0 = 2$ msec [10]	Gettered Metal/SiO ₂ /Si (MOS) capacitors
10^{-6} – 10^{-4} sec	$\tau_n = 23.5$ μ sec $\tau_p = 1.5$ μ sec [11]	<i>pn</i> -junction devices
10^{-8} – 10^{-6} sec	$\tau_n = 0.75$ μ sec $\tau_p = 0.25$ μ sec [11]	Au-diffused <i>pn</i> -junction devices

$$\downarrow \tau_n = \frac{1}{\nu_{th} \sigma \frac{N_T}{2}}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



LOW LEVEL INJECTION



- Low level injection:
 - changes in the carrier concentrations are much less than the majority carrier concentration under equilibrium conditions
 - $\Delta n = n - n_0$ and $\Delta p = p - p_0$
 - $\Delta n, \Delta p \ll n_0$ (n-type material), $\Delta n, \Delta p \ll p_0$ (p-type material)
- Assumptions about the R-G center parameters
 - R-G centers introduce E_T ' level close to midgap $\rightarrow n_1 \sim p_1 \sim n_i$,
 - R-G center concentration is sufficiently low $\rightarrow \Delta n \sim \Delta p$
 - τ_n and τ_p are taken to differ by no more than a few orders of magnitude
- Low level injection
 - $R = \Delta n / \tau_n$ (p-type); $R = \Delta p / \tau_p$ (n-type);
- High level injection
 - $R = \Delta p / (\tau_p + \tau_n)$ where $\Delta n, \Delta p \gg n_0$ or p_0

$$R = \frac{(n_0 + \Delta n)(p_0 + \Delta p) - n_i^2}{\tau_p(n_0 + \Delta n + n_1) + \tau_n(p_0 + \Delta p + p_1)}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



RG DEPLETION AND CAPTURE CROSS-SECTION



- Electrostatic depletion region:
 - $n, p \ll |N_D - N_A|$, does not imply carrier deficit
 - System in equilibrium $\rightarrow n = n_0, p = p_0$ and $np = n_i^2$
- R-G depletion defined as :
 - semiconductor volume where $n \ll n_1$ and $p \ll p_1$
 - $np \ll n_1 p_1 = n_i^2$, deficit of carriers
 - $R = \frac{-n_i^2}{\tau_p n_1 + \tau_n p_1} = -\frac{n_i}{\tau_0}$ where $\tau_0 = \tau_n + \tau_p$ if $E_T' = E_i$

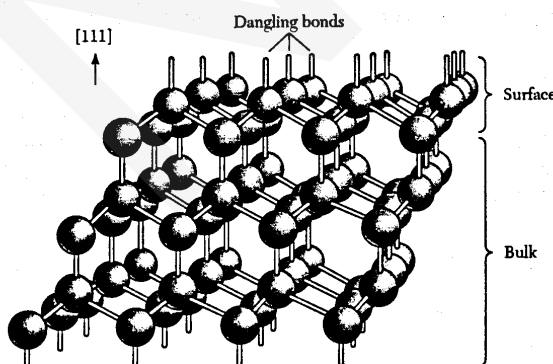
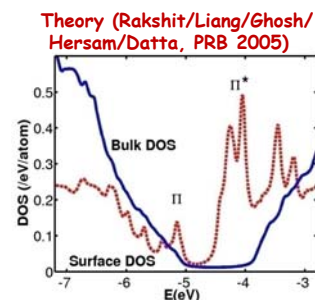
SEMICONDUCTOR DEVICE MODELING AND SIMULATION



SURFACE RECOMBINATION



- Lattice periodicity broken at surface/interface - mid-gap E levels
- Carriers generated-recombined per unit area
- Processes and descriptions analogous to bulk R-G using surface parameters



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SURFACE RECOMBINATION



- For a **single energy level** surface state:

$$\begin{aligned} r_N &= c_n(p_T n - n_T n_1) & \longrightarrow & r_{Ns} = c_{ns}(p_{Ts} n_s - n_{Ts} n_{1s}) \\ r_P &= c_p(n_T p - p_T p_1) & \longrightarrow & r_{Ps} = c_{ps}(n_{sT} p_s - p_{Ts} p_{1s}) \end{aligned}$$

$$\begin{aligned} n_1 &= n_i e^{(E'_T - E_i)/kT} & \longrightarrow & n_{1s} = n_i e^{(E'_{iT} - E_i)/kT} \\ p_1 &= p_i e^{(E_i - E'_T)/kT} & \longrightarrow & p_{1s} = p_i e^{(E_i - E'_{iT})/kT} \end{aligned}$$

$$R = \frac{np - n_i^2}{\tau_p(n + n_1) + \tau_n(p + p_1)} \quad \longrightarrow \quad R = \frac{n_s p_s - n_i^2}{\frac{1}{s_p}(n_s + n_{1s}) + \frac{1}{s_n}(p_s + p_{1s})}$$

Surface recombination velocities $s_p \equiv c_{ps} N_{Ts}$ and $s_n \equiv c_{ns} N_{Ts}$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

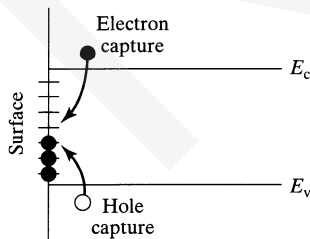


MULTI-LEVEL (MORE REALISTIC)

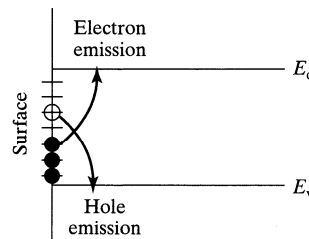


$D_{IT}(E)$ - density of interface traps (per unit area-energy)
 $D_{IT}(E)dE$ - density of IT between E and $E+dE$ (replaces N_{Ts})

$$R = \int_{E_v}^{E_c} \frac{n_s p_s - n_i^2}{\frac{1}{c_{ps}}(n_s + n_{1s}) + \frac{1}{c_{ns}}(p_s + p_{1s})} D_{IT}(E) dE$$



(a) Capture



(b) Emission

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CONCLUSION



- Discussed optical absorption, surface recombination and derived SRH recombination

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Thank you



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SEMICONDUCTOR DEVICE MODELING AND SIMULATION

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Indian Institute of Technology Kharagpur

SOLUTION TO DD EQUATIONS

LECTURE: 46



L46 RECALL DD EQUATIONS



Poisson equation

$$\frac{d^2 \psi}{dx^2} = -\frac{\rho}{\epsilon} = -\frac{q}{\epsilon} (p - n + N_D^+ - N_A^-)$$

$$\frac{d}{dx} \left(\epsilon \frac{d\psi}{dx} \right) = -\rho = -q(p - n + N_D^+ - N_A^-)$$

Handwritten notes: $V(\psi) = \phi$, $\epsilon = \epsilon_0 \epsilon_r$

Carrier density equations

$$n = n_i \cdot \exp\left(\frac{E_F - E_i}{k_B T}\right) = n_i \cdot \exp\left(\frac{q(\psi - \phi_n)}{k_B T}\right) = n_i \cdot \exp\left(\frac{V}{V_T}\right)$$

$$p = n_i \cdot \exp\left(\frac{E_i - E_F}{k_B T}\right) = n_i \cdot \exp\left(\frac{q(\phi_p - \psi)}{k_B T}\right) = n_i \cdot \exp\left(-\frac{V}{V_T}\right)$$

Continuity equations

$$\frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} + G_n - R_n$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} \frac{\partial J_p}{\partial x} + G_p - R_p$$

Handwritten notes: $J_n = qn\mu_n E$, $J_p = -qp\mu_p E$

current density equations

$$\bar{J}_n = -qn\mu_n \frac{\partial \psi}{\partial x} + qD_n \frac{\partial n}{\partial x}$$

$$\bar{J}_p = -qp\mu_p \frac{\partial \psi}{\partial x} - qD_p \frac{\partial p}{\partial x}$$

Recombination rate equation

$$R = R_n = R_p = \frac{np - n_i^2}{\tau_p(n + n_i) + \tau_n(p + p_i)} = \frac{np - n_i^2}{n + p + 2n_i \cosh\left(\frac{E_T - E_i}{k_B T}\right)} \frac{1}{\tau}$$

Handwritten notes: ψ, p, n , ψ, ϕ_p, ϕ_n , $E_T - E_i$, E_F , E_V

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

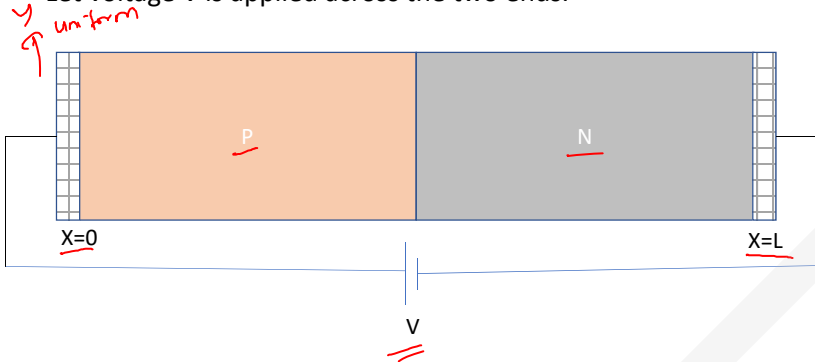


PROBLEM



Consider a P-N junctions with uniform cross-section so that the problem is one dimensional

Let voltage V is applied across the two ends.



$$n = n_i \exp\left(\frac{E_F - E_i}{k_B T}\right) = n_i \exp\left(\frac{q(\psi - \phi_n)}{k_B T}\right)$$

$$p = n_i \exp\left(\frac{E_i - E_F}{k_B T}\right) = n_i \exp\left(\frac{q(\phi_p - \psi)}{k_B T}\right)$$

$$E_F = -q\phi_n$$

$$E_i = -q\phi$$

Unknowns:

n, p, ψ

OR

ψ, ϕ_n, ϕ_p

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



BOUNDARY CONDITIONS



Consider a P-N junctions with uniform cross-section so that the problem is one dimensional

Let voltage V is applied across the two ends.



$$\frac{d^2\psi}{dx^2} = -\frac{\rho}{\epsilon} = -\frac{q}{\epsilon}(p - n + C), \quad C = N_D^+ - N_A^-$$

Ohmic contact at $x=0$ and $x=L \rightarrow$ space charge should be zero



Physical boundary: contact and interface to insulator

- Ohmic-no potential drop $V_{app} = \psi - \psi_{built-in}$
- Schottky $V_{app} = \psi - \psi_{built-in} + \psi_{Schottky_Barrier}$
- Interface to Insulating material

Artificial boundaries

- To separate neighboring devices
- To simplify numerical solution

$$\epsilon_{sc} \frac{\partial \psi}{\partial n} \bigg|_{sc} - \epsilon_{ins} \frac{\partial \psi}{\partial n} \bigg|_{ins} = Q_{int}$$

$$\psi = \psi_{sc} \text{ or } \psi = \psi_{ins}$$

$$\frac{\partial \psi}{\partial n} = 0$$

$$\frac{\partial n}{\partial x} = 0$$

$$\frac{\partial p}{\partial x} = 0$$

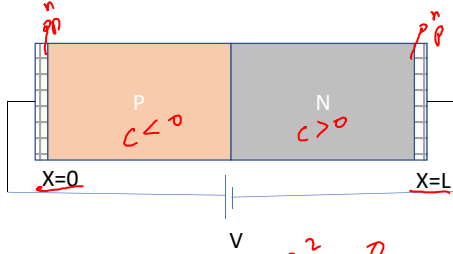
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BOUNDARY CONDITIONS



Consider a P-N junctions with uniform cross-section so that the problem is one dimensional
Let voltage V is applied across the two ends.



$$\frac{d^2\psi}{dx^2} = -\frac{\rho}{\epsilon} = -\frac{q}{\epsilon}(p-n+C), \quad C = N_D^+ - N_A^-$$

Ohmic contact at $x=0$ and $x=L \rightarrow$ space charge should be zero

$$C(0) + p(0) - n(0) = 0$$

$$C(L) + p(L) - n(L) = 0$$

$$p(0) \times n(0) = n_i^2$$

$$p(L) \times n(L) = n_i^2$$

$$p(0) = \frac{-C \pm \sqrt{C^2 + 4n_i^2}}{2}$$

$$n(L) = \frac{C \pm \sqrt{C^2 + 4n_i^2}}{2}$$

$$n(0) = \frac{n_i^2}{p(0)}$$

$$p(L) = \frac{n_i^2}{n(L)}$$

$$\begin{aligned} C + p - \frac{n_i^2}{p} &= 0 \\ p^2 + Cp - n_i^2 &= 0 \\ p &= \frac{-C \pm \sqrt{C^2 + 4n_i^2}}{2} \end{aligned}$$

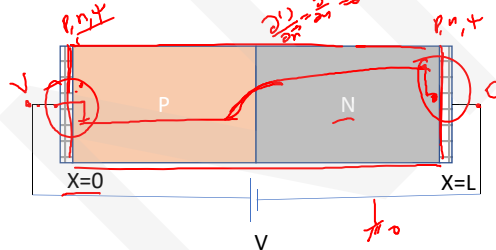
SEMICONDUCTOR DEVICE MODELING AND SIMULATION



BOUNDARY CONDITIONS



Consider a P-N junctions with uniform cross-section so that the problem is one dimensional
Let voltage V is applied across the two ends.



$$\frac{d^2\psi}{dx^2} = -\frac{\rho}{\epsilon} = -\frac{q}{\epsilon}(p-n+C), \quad C = N_D^+ - N_A^-$$

Ohmic contact at $x=0$ and $x=L \rightarrow$ space charge should be zero

$$C(0) + p(0) - n(0) = 0$$

$$C(L) + p(L) - n(L) = 0$$

$$p(0) \times n(0) = n_i^2$$

$$p(L) \times n(L) = n_i^2$$

$$\psi(0) = V - \frac{k_B T}{q} \ln \left[\frac{p(0)}{n_i} \right]$$

$$\psi(L) = 0 + \frac{k_B T}{q} \ln \left[\frac{n(L)}{n_i} \right]$$

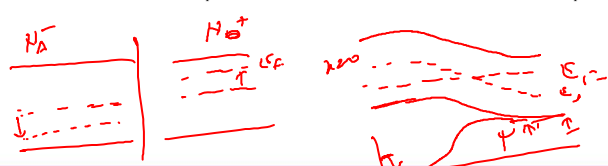
$$E_F = -q\phi_n(0) = -q\phi_p(0) = -qV$$

$$E_F = -q\phi_n(L) = -q\phi_p(L) = -q \cdot 0$$

$$V_{app} = \psi - \psi_{built-in}$$

$$\psi_{built-in} = \psi - \phi_n \text{ or } \psi - \phi_p$$

$$\begin{aligned} \psi(0) &= V_{app} + \psi_{built-in} \\ \psi(0) &= 0 + \psi_{built-in} \\ \psi(0) &= V + \psi_{built-in} \end{aligned}$$



SEMICONDUCTOR DEVICE MODELING AND SIMULATION

DISCRETIZATION AND SCALING

Poisson equation

$$\frac{d^2\psi}{dx^2} = -\frac{\rho}{\epsilon} = -\frac{q}{\epsilon} (p - n + N_D^+ - N_A^-)$$

Discretization

$$\frac{-\epsilon}{n_i q} \frac{\psi(x_{i-1}) - 2\psi(x_i) + \psi(x_{i+1}))}{(h_x)^2} - \exp\left(\frac{q(\phi_p(x_i) - \psi(x_i))}{k_B T}\right) + \exp\left(\frac{q(\psi(x_i) - \phi_n(x_i))}{k_B T}\right) - \frac{C(x_i)}{n_i} = 0$$

Scaling

$$\lambda^2 \frac{\tilde{\psi}(i-1) - 2\tilde{\psi}(i) + \tilde{\psi}(i+1))}{(\tilde{h}_x)^2} - \exp(\tilde{\phi}_p(i) - \tilde{\psi}(i)) + \exp(\tilde{\psi}(i) - \tilde{\phi}_n(i)) - \tilde{C}(i) = 0$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

DISCRETIZE EQUATIONS

current density equations

$$\bar{J}_n = -qn\mu_n \frac{\partial \psi}{\partial x} + qD_n \frac{\partial n}{\partial x}$$

$$\bar{J}_p = -qp\mu_p \frac{\partial \psi}{\partial x} - qD_p \frac{\partial p}{\partial x}$$

Discretized Equations

$$\bar{J}_p(i+1/2) = -q \frac{p(i) + p(i+1)}{2} \mu_p(i+1/2) \frac{\psi(i+1) - \psi(i)}{h} - qD_p(i+1/2) \frac{p(i+1) - p(i)}{h}$$

$$\bar{J}_p(i-1/2) = -q \frac{p(i-1) + p(i)}{2} \mu_p(i-1/2) \frac{\psi(i) - \psi(i-1)}{h} - qD_p(i-1/2) \frac{p(i) - p(i-1)}{h}$$

Boundary Conditions

$$\left\{ \begin{array}{l} \frac{\mu_p(M-1)}{2h(M-1)} \left[\frac{2}{\theta} + \psi(N-1) - \psi(N) \right] \cdot p(N-1) + \\ \left[\frac{\mu_p(M-1)}{2h(M-1)} \left[\frac{2}{\theta} - \psi(N-1) + \psi(N) \right] \dots \right] \cdot p(N) \\ + \frac{\mu_p(M)}{2h(M)} \left[\frac{2}{\theta} + \psi(N) - \psi(N+1) \right] \cdot p(N+1) \end{array} \right\}$$

$$+ \frac{\mu_p(M)}{2h(M)} \left[\psi(N) - \psi(N+1) - \frac{2}{\theta} \right] \cdot p(N+1) = h'(N) [G(N) - U(N)]$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



DISCRETIZE EQUATIONS



current density equations- Scharfetter-Gummel Discretization

$$\bar{J}_n = -qn\mu_n \frac{\partial \psi}{\partial x} + qD_n \frac{\partial n}{\partial x}$$

$$\bar{J}_p = -qp\mu_p \frac{\partial \psi}{\partial x} - qD_p \frac{\partial p}{\partial x}$$

$$J_{i+1/2}^n = \frac{eD_{i+1/2}^n}{\Delta} [n_{i+1} B(\frac{\Psi_{i+1} - \Psi_i}{V_t}) - n_i B(\frac{\Psi_i - \Psi_{i+1}}{V_t})]$$

$$B(x) = \frac{x}{e^x - 1}$$

$$J_n(i+1/2) = \frac{q}{h_x} [A_1 n(i+1) + A_2 n(i)]$$

$$A_1 = D(i+1/2) B(\frac{\psi(i+1) - \psi(i)}{k_B T / q}) = \mu_p(i+1/2) \cdot \frac{\psi(i+1) - \psi(i)}{\exp(q(\psi(i+1) - \psi(i)) / k_B T) - 1}$$

$$A_2 = D(i+1/2) B(\frac{\psi(i) - \psi(i+1)}{k_B T / q}) = \mu_p(i+1/2) \cdot \frac{\psi(i) - \psi(i+1)}{\exp(q(\psi(i) - \psi(i+1)) / k_B T) - 1}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



DISCRETIZE EQUATIONS



Continuity equations

$$\frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} + G_n - R_n$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} \frac{\partial J_p}{\partial x} + G_p - R_p$$

$$\frac{1}{q} \frac{J_p(i+1/2) - J_p(i-1/2)}{h(i)} - G(i) + R(i) = 0$$

$$\frac{1}{q} \frac{J_n(i+1/2) - J_n(i-1/2)}{h(i)} + G(i) - R(i) = 0$$

$$n = n_i \cdot \exp(\frac{E_F - E_i}{k_B T}) = n_i \cdot \exp(\frac{q(\psi - \phi_n)}{k_B T}) = n_i \cdot \exp(\frac{V}{V_t})$$

$$p = n_i \cdot \exp(\frac{E_i - E_F}{k_B T}) = n_i \cdot \exp(\frac{q(\phi_p - \psi)}{k_B T}) = n_i \cdot \exp(-\frac{V}{V_t})$$

$$\frac{D_{i+1/2}^n}{\Delta^2} B(\frac{\Psi_{i+1} - \Psi_i}{V_t}) n_{i+1} - n_i [\frac{D_{i-1/2}^n}{\Delta^2} B(\frac{\Psi_i - \Psi_{i-1}}{V_t}) + \frac{D_{i+1/2}^n}{\Delta^2} B(\frac{\Psi_i - \Psi_{i+1}}{V_t})] + \frac{D_{i-1/2}^n}{\Delta^2} B(\frac{\Psi_{i-1} - \Psi_i}{V_t}) n_{i-1} = G_i$$

$$B(x) = \frac{x}{e^x - 1}$$

$$\frac{D_{i-1/2}^p}{\Delta^2} B(\frac{\Psi_i - \Psi_{i-1}}{V_t}) p_{i-1} - p_i [\frac{D_{i-1/2}^p}{\Delta^2} B(\frac{\Psi_{i-1} - \Psi_i}{V_t}) + \frac{D_{i+1/2}^p}{\Delta^2} B(\frac{\Psi_{i+1} - \Psi_i}{V_t})] + \frac{D_{i+1/2}^p}{\Delta^2} B(\frac{\Psi_i - \Psi_{i+1}}{V_t}) p_{i+1} = G_i$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



NUMERICAL SOLUTION APPROACH



- Poisson solvers:
 - Direct
 - Gaussian Elimination
 - LU decomposition
 - Iterative
 - Mesh Relaxation Methods
 - Jacobi, Gauss-Seidel, Successive over-Relaxation
 - Advanced Iterative Solvers
 - ILU, Stone's strongly implicit method, Conjugate gradient methods and Multigrid methods
- Solution Procedures:
 - Gummel's Approach – when the constitutive equations are weakly coupled
 - Newton's Method – when the constitutive equations are strongly coupled
 - Gummel/Newton – more efficient approach

$$\begin{array}{r}
 Ax = b \\
 \hline
 Lx \approx b \\
 \hline
 Lx = b \\
 \hline
 Ux = y
 \end{array}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



CONCLUSION



- Discussed technique to solving DD equations
- discretization of the semiconductor equations yields a large system of nonlinear algebraic equations
- In case of DD there are three equations (one Poisson and two continuity equations)

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A slide with a yellow and blue header. The NPTEL logo is on the left, and the text "NPTEL ONLINE CERTIFICATION COURSE" is in the center. The IIT Kharagpur logo is on the right. Below the header, there is a large photograph of the IIT Kharagpur campus. On the right side, there is a purple box containing the course title and lecturer information. At the bottom left, there is a white box containing the lecture title and number.

NPTEL ONLINE CERTIFICATION COURSE

**SEMICONDUCTOR DEVICE
MODELING AND SIMULATION**

PROF. VIVEK DIXIT
Department of Electronics and Electrical Communication
Engineering
Indian Institute of Technology Kharagpur

SOLUTION TO NONLINEAR
ALGEBRAIC EQUATIONS

LECTURE: 47



L47 NONLINEAR ALGEBRAIC EQUATIONS



Consider set of three equations

$$F(\psi) = F(\psi, n, p) = \begin{pmatrix} F_1(\psi, n, p) \\ F_2(\psi, n, p) \\ F_3(\psi, n, p) \end{pmatrix}$$

Poisson
continuity
Coupled

Set of unknowns

$$w = \begin{pmatrix} \psi \\ n \\ p \end{pmatrix}$$

only iterative methods are applicable for the solution of systems of nonlinear algebraic equations

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



ITERATIVE (NEWTON) METHODS



Let us solve algebraic equation $f(x)=0$ with initial guess x^0

Let us $x^{(1)}$ is k^{th} estimate.

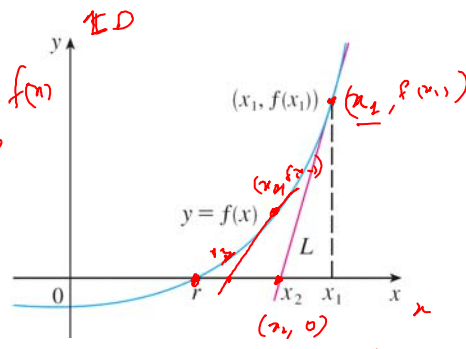
$x^{(2)}$ is $K+1^{\text{st}}$ estimate, can be evaluated as

$$x^{(2)} = x^{(1)} - \frac{f(x^{(1)})}{\partial f(x^{(1)}) / \partial x} = x^{(1)} - \frac{f(x^{(1)})}{f'(x^{(1)})}$$

$$x^{(3)} = x^{(2)} - \frac{f(x^{(2)})}{f'(x^{(2)})}$$

$$\frac{V=0.2}{5.01 \times 10^{-12} \times 10^{-12}} \times \frac{1}{10^{-12}}$$

$$f(x) = 0$$



$$x_1 \leftarrow x_2 = \frac{f(x_1)}{(\frac{\partial f}{\partial x})_{x_1}}$$

$$\frac{f(x_1) - 0}{x_1 - x_2} = \frac{\partial f}{\partial x} \bigg|_{x=x_1}$$

$$x_2 = x_1 - \frac{f(x_1)}{(\frac{\partial f}{\partial x})_{x_1}}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



ITERATIVE (NEWTON) METHODS



Let us solve algebraic equation $f(x)=0$ with initial guess x^0

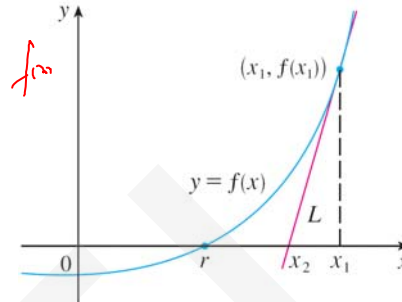
Let us $x^{(1)}$ is k^{th} estimate.

$x^{(2)}$ is $K+1^{\text{st}}$ estimate, can be evaluated as

$$x^{(2)} = x^{(1)} - \frac{f(x^{(1)})}{\partial f(x^{(1)}) / \partial x}$$

$$\delta x = \frac{f(x)}{f'(x)}$$

$$f(x+1) = f(x) + \delta x \cdot f'(x)$$



The idea behind Newton's method is that the tangent line is close to the curve and so its x-intercept is close to the x-intercept of the curve ($r = \text{root}$)

$$\delta x^{(k)} = \frac{f(x^{(k)})}{\partial f(x^{(k)}) / \partial x}$$

$$\partial f(x^{(k)}) / \partial x \cdot \delta x^{(k)} = f(x^{(k)})$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



ITERATIVE (NEWTON) METHOD THEORY



Assume that a solution w^* exists for the system of equations and there exists a neighbourhood of w^* within which no other solution exists

All iterative methods are based on a fixpoint equation

$$w = M(w)$$

fixpoint equation is used directly for iteration $w^{(k+1)} = M(w^{(k)})$

$$w^{(k+1)} = M(w^{(k)}) = w^{(k)} - B(w^{(k)})^{-1} \cdot F(w^{(k)})$$

$$M'(w) = I - (B(w)^{-1})' \cdot F(w) - B(w)^{-1} \cdot F'(w)$$

requirements on $B(w)$ such that the iterative scheme converges. variety of operators $B(w)$ exists to satisfy the equation

$$M'(w^*) = I - B(w^*)^{-1} \cdot F'(w^*)$$

The classical Newton method is defined by

$$B(w^*) = F'(w^*)$$

$$M = I - \frac{F'}{F} = 0$$

$$f(w, p, n) = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \end{bmatrix} = 0$$

$$w = \begin{bmatrix} \psi \\ p \\ n \end{bmatrix} - \text{unknowns}$$

$$w = M(w)$$

$$\psi = \begin{bmatrix} \psi \\ p \\ n \end{bmatrix}$$

$$f(x) = 0$$

$$f = w - \text{new} = 0$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



ITERATIVE (NEWTON) METHODS



Initial guess $w^0 = \begin{pmatrix} \psi^0 \\ n^0 \\ p^0 \end{pmatrix}$

Correction for k^{th} iteration

$$\delta w^k = w^{k+1} - w^k = \begin{pmatrix} \psi^{k+1} \\ n^{k+1} \\ p^{k+1} \end{pmatrix} - \begin{pmatrix} \psi^k \\ n^k \\ p^k \end{pmatrix}$$

Extending idea to higher dimensions
Newton's method at the k^{th} step

Finite-difference

Jacobian

$$\begin{pmatrix} \frac{\partial F_1}{\partial \psi} & \frac{\partial F_1}{\partial n} & \frac{\partial F_1}{\partial p} \\ \frac{\partial F_2}{\partial \psi} & \frac{\partial F_2}{\partial n} & \frac{\partial F_2}{\partial p} \\ \frac{\partial F_3}{\partial \psi} & \frac{\partial F_3}{\partial n} & \frac{\partial F_3}{\partial p} \end{pmatrix} \cdot \begin{pmatrix} \delta \psi^k \\ \delta n^k \\ \delta p^k \end{pmatrix} = - \begin{pmatrix} F_1(\psi^k, n^k, p^k) \\ F_2(\psi^k, n^k, p^k) \\ F_3(\psi^k, n^k, p^k) \end{pmatrix}$$

ϕ_n, ϕ_p

$$\delta w = -F$$

$$\delta w = -J^{-1} F$$

$$\frac{\partial F_1}{\partial \psi} \delta \psi + \frac{\partial F_1}{\partial n} \delta n + \frac{\partial F_1}{\partial p} \delta p = -F_1(\psi, n, p)$$

$$\frac{\partial F_1}{\partial \psi} \delta \psi = -F_1$$

$$\delta \psi = -\frac{F_1}{(\partial F_1 / \partial \psi)}$$

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BLOCK-NEWTON METHOD



block iteration scheme (iteration index m) for the solution of the k -th Newton step

$$\begin{pmatrix} \frac{\partial F_1}{\partial \psi} & 0 & 0 \\ \frac{\partial F_2}{\partial \psi} & \frac{\partial F_2}{\partial n} & 0 \\ \frac{\partial F_3}{\partial \psi} & \frac{\partial F_3}{\partial n} & \frac{\partial F_3}{\partial p} \end{pmatrix}^k \cdot \begin{pmatrix} \delta \psi^k \\ \delta n^k \\ \delta p^k \end{pmatrix}^{m+1} = - \begin{pmatrix} F_1(\psi^k, n^k, p^k) \\ F_2(\psi^k, n^k, p^k) \\ F_3(\psi^k, n^k, p^k) \end{pmatrix} - \begin{pmatrix} 0 & \frac{\partial F_1}{\partial n} & \frac{\partial F_1}{\partial p} \\ 0 & 0 & \frac{\partial F_2}{\partial p} \\ 0 & 0 & 0 \end{pmatrix}^k \cdot \begin{pmatrix} \delta \psi^k \\ \delta n^k \\ \delta p^k \end{pmatrix}^m$$

$$\frac{\partial F_1}{\partial \psi} \delta \psi^k = -F_1(\psi^k, n^k, p^k) - \frac{\partial F_1}{\partial n} \delta n^k - \frac{\partial F_1}{\partial p} \delta p^k$$

$$-F_1(\psi, n, p - \delta p)$$

coefficient matrix is block lower triangular, one can decouple the system into three linear systems which **can be solved sequentially**

$$w = M(w)$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



SOR BLOCK-NEWTON METHOD



Successive over relaxation

block iteration scheme (iteration index m) for the solution of the k-th Newton step

$$\begin{pmatrix} \frac{\partial F_1}{\partial \psi} & 0 & 0 \\ \frac{\partial F_2}{\partial \psi} & \frac{\partial F_2}{\partial n} & 0 \\ \frac{\partial F_3}{\partial \psi} & \frac{\partial F_3}{\partial n} & \frac{\partial F_3}{\partial p} \end{pmatrix}^k \cdot \begin{pmatrix} \delta \psi^k \\ \delta n^k \\ \delta p^k \end{pmatrix}^{m+1} = -\omega \begin{pmatrix} F_1(\psi^k, n^k, p^k) \\ F_2(\psi^k, n^k, p^k) \\ F_3(\psi^k, n^k, p^k) \end{pmatrix} - \omega \begin{pmatrix} 0 & \frac{\partial F_1}{\partial n} & \frac{\partial F_1}{\partial p} \\ 0 & 0 & \frac{\partial F_2}{\partial p} \\ 0 & 0 & 0 \end{pmatrix}^k \cdot \begin{pmatrix} \delta \psi^k \\ \delta n^k \\ \delta p^k \end{pmatrix}^m$$

ω is relaxation parameter.

$$\frac{\partial F_1}{\partial \psi} \delta \psi^{km+1} = -\omega \cdot F_1(\psi^k, n^k + \delta n^{km}, p^k + \delta p^{km})$$

$$\frac{\partial F_2}{\partial n} \delta n^{km+1} = -\omega \cdot F_1(\psi^k + \delta \psi^{km+1}, n^k, p^k + \delta p^{km})$$

$$\frac{\partial F_3}{\partial p} \delta p^{km+1} = -\omega \cdot F_1(\psi^k + \delta \psi^{km+1}, n^k + \delta n^{km+1}, p^k)$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



DIRECT METHOD



Direct methods are used for sparse matrices. All direct methods for the solution of sparse systems of linear equations are based on variants of Gaussian elimination

$$Ax = b$$

All methods factorization the coefficient matrix A to the form:

$$P.A.Q = L.U$$

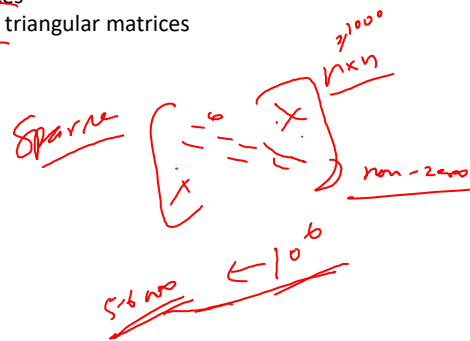
P and Q are permutation matrices

L and U is a lower and an upper triangular matrices

For symmetrical coefficient matrix A :

$$P.A.P^T = L.D.L^T$$

D is a diagonal matrix



SEMICONDUCTOR DEVICE MODELING AND SIMULATION

GAUSS ELIMINATION-EXAMPLE

$$\begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \\ -6 \end{bmatrix}$$

A *b*

Matlab Program to solve $Ax=b$ using Gaussian Elimination method

```

clear ; clc ; close all
A = [ 1 2 -1 ; 2 1 -2 ; -3 1 1 ];
b = [ 3 3 -6 ]';
n=3; %size of eqns
x=zeros(n,1);
if det(A) == 0
    disp('Solution does not exist')
    return
end
M = [ A b ]
for i = 1:(n-1)
    for j = (i+1) : n
        M(j,:) = M(j,:) - M(i,:)*M(j,i)/M(i,i);
    end
end
x(p) = M(p,n+1)/M(p,p) - sum_{r=p+1}^n x(r)*M(p,r)/M(p,p)

```

Handwritten notes:

- $x_1 + 2x_2 - x_3 = 3$
- $2x_1 + x_2 - 2x_3 = 3$
- $-3x_1 + x_2 + x_3 = -6$
- Augmented matrix: $\begin{bmatrix} 1 & 2 & -1 & 3 \\ 2 & 1 & -2 & 3 \\ -3 & 1 & 1 & -6 \end{bmatrix}$
- Row operations: $R_2 \rightarrow R_2 - 2R_1$, $R_3 \rightarrow R_3 + 3R_1$
- Resulting matrix: $\begin{bmatrix} 1 & 2 & -1 & 3 \\ 0 & -3 & 0 & -3 \\ 0 & 7 & -2 & 15 \end{bmatrix}$
- Final solution: $x = \begin{bmatrix} 3 \\ 1 \\ 2 \end{bmatrix}$

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CONCLUSION

- Discussed Newton based iterative solving methods and direct method for sparse matrices

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PROBLEM-1



$$\begin{aligned}\bar{J}_{n,drift} &= qn\mu_n E = -n\mu_n \bar{F}_e \\ \bar{J}_{n,diff} &= qD_n \nabla_r n\end{aligned}$$

Equating

$$D_n / \mu_n = -n \bar{F}_e / (q \nabla_r n)$$

For isothermal solid with parabolic band structure, Force = $-dE_F/dx$
 $D/\mu = (n/q) dE_F/dn = (1/q) dE_F/d(\ln n)$

For non-degenerate semiconductors, $n = n_i \exp((E_F - E_i)/kT)$
 $d(\ln n)/dE_F = 1/kT$
 $D/\mu = kT/q$

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PROBLEM-2



The Hall effect can be used to determine the type of carriers present in a material. Show that the Hall constant R is given by

$$R = -\frac{1}{qn_i} \frac{\mu_n / \mu_p - 1}{\mu_n / \mu_p + 1} = -\frac{1}{2n_i} \frac{\mu_n - \mu_p}{\mu_n + \mu_p}$$

for an intrinsic semiconductor, where n_i is the intrinsic carrier concentration and μ_n and μ_p are the electron and hole mobilities.

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



PROBLEM-2: Recall Hall Effect



(p-type material)

- $\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$ (Lorentz force)
- Net force in y-axis: $F_y = q(\mathcal{E}_y - v_x B_z)$

- 0 current in y-direction
- $\rightarrow \mathcal{E}_y = v_x B_z$
- $\mathcal{E}_y = (J_x / qp_0) B_z = R_H J_x B_z$
- Hall voltage
- $V_{AB} = \mathcal{E}_y w$
- Hall coefficient
- $R_H = \mathcal{E}_y / J_x B_z = 1 / qp_0$

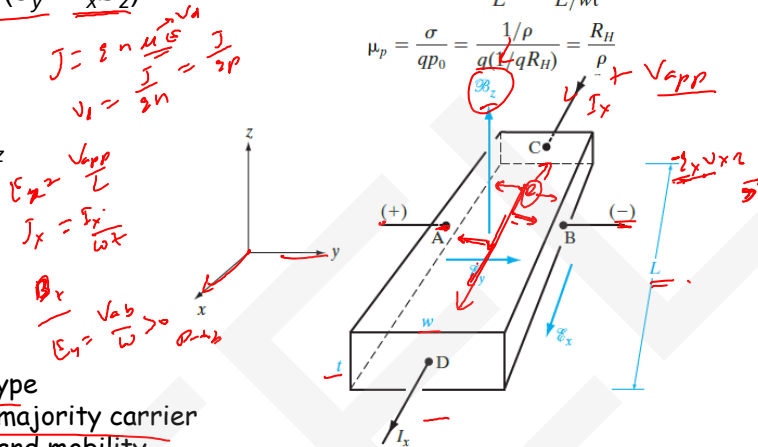
- $V_{AB} < 0$ for n-type
- R_H and ρ yield majority carrier concentration and mobility

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

$$\rho_0 = \frac{1}{qR_H} = \frac{J_x B_z}{q \mathcal{E}_y} = \frac{(I_x / wt) B_z}{q(V_{AB} / w)} = \frac{I_x B_z}{qV_{AB}}$$

$$\rho(\Omega - \text{cm}) = \frac{Rwt}{L} = \frac{V_{CD} / I_x}{L / wt}$$

$$\mu_p = \frac{\sigma}{qp_0} = \frac{1/\rho}{qR_H} = \frac{R_H}{\rho}$$



PROBLEM-2: Recall Hall Effect



Hall effect (general)

- $F_{hy} = eE_y - ev_{hx} B_z = ev_{hy} / \mu_h$
- $-F_{ey} = eE_y + ev_{ex} B_z = ev_{ey} / \mu_e$
- $J_y = epv_{hy} + env_{ey} = 0$
- $J_x = epv_{hx} + env_{ex}$
- $R_H = E_y / J_x B_z$

$$R_H = \frac{p\mu_h^2 - n\mu_e^2}{e(p\mu_h + n\mu_e)^2}$$

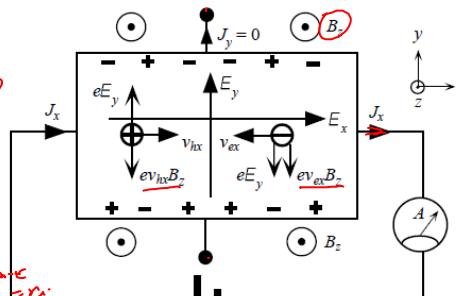
$$= \frac{n_i^2 (\mu_h^2 - \mu_e^2)}{en_i^2 (p\mu_h + n\mu_e)^2}$$

$$R_H = \frac{\mu_h - \mu_e}{e n_i (\mu_h + \mu_e)}$$

- accurate expression including Hall scattering factor r_e and r_h using ($J_y = r_e epv_{hy} + r_h env_{ey} = 0$),

$$R_H = \frac{r_h p - r_e b^2 n}{e(p + bn)^2}, \quad b = \frac{\mu_e}{\mu_h}$$

DEVICE MODELING AND SIMULATION



$$v = \mu E = \frac{m}{e} \frac{F}{m} = \frac{e}{m} F$$

$$J = \left(b \mu_h \mu_e \right) (E)$$

$$v_{hx} = \mu_h E_y$$

$$v_{hx} = \mu_e E_x$$



PROBLEM-3: Include Hall Scattering effect



$$R_H = \frac{p\mu_h^2 - n\mu_e^2}{e(p\mu_h + n\mu_e)^2}$$

General expression including Hall scattering factor r_e and r_h using ($J_y = r_e p v_{hy} + r_h n v_{ey} = 0$),

$$R_H = \frac{r_h p - r_e b^2 n}{e(p + b n)^2}$$

- $r_H = (r_e \sim r_h) = \mu_H / \mu_C = \frac{\langle \tau_m^2 \rangle}{\langle \tau_m \rangle^2}$ Handwritten: $\mu_C = \frac{e \hbar^2}{m}$
- Hall mobility, $\mu_H = r_H \mu$ ($\sim$ drift mobility) Handwritten: $\mu_H \propto \frac{1}{\sqrt{E}}$
- For semiconductor with spherical constant-energy surfaces, $\tau_m \propto E^{-1/2}$ for phonon scattering and $\tau_m \propto E^{-3/2}$ for ionized impurity scattering
- $\langle \tau_m^2 \rangle = \int_0^\infty \tau_m^2 E^{3/2} \exp\left(-\frac{E}{kT}\right) dE / \int_0^\infty E^{3/2} \exp\left(-\frac{E}{kT}\right) dE$
- $r_H = 3\pi/8 = 1.18$ for phonon scattering and $r_H = 315\pi/512 = 1.93$ for ionized impurity scattering.
- Magnetoresistance effect: under strong magnetic field significant increase in resistivity is observed due to carriers traveling in a path that deviates from the applied electric field.



SEMICONDUCTOR DEVICE MODELING AND SIMULATION



PROBLEM-4



Solve poisson equation 2D : $-\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = 20 \cos(3\pi x) \times \sin(2\pi y)$ for $x = [0, 1]; y = [0, 1]$

Dirichlet boundary (left and right edge)

$$u(x=0) = 0$$

$$u(x=1) = 1$$

Neumann boundary for y-axis $\frac{\partial u}{\partial n} = 0 = \frac{\partial u}{\partial y}$ (upper and lower edge)

%--Define the 2D mesh

loop=1;

N=20; Nx=N; Ny=N;

xa=0; xb=1; ya=0; yb=1;

dx=(xb-xa)/(Nx-1);

dy=(yb-ya)/(Ny-1);

%% since $dx = dy$ we can use $h = dx = dy$

h=dx;

M=400; % maximum iteration value

%--Initialize

V(1:Nx,1:Ny)=0.0;

f(1:Nx,1:Ny)=0.0;

for i=1:Nx,

for j=1:Ny,

f(i,j)=20*cos(3*pi*(xa+(i-1)*dx))*sin(2*pi*(ya+(j-1)*dy));

end

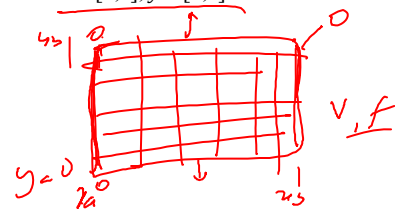
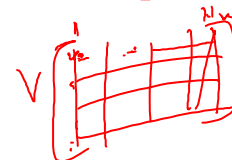
End

% Boundary conditions

V(1,:)=0;

V(Nx,:)=1; %% Dirichlet in x

g=0; %% Neumann in y



SEMICONDUCTOR DEVICE MODELING AND SIMULATION

PROBLEM-4

```

w=cos(pi/Nx)+cos(pi/Ny); % Converging Term
Ncount=0;
loop=1;
while loop==1;
    Rmin=0;
    j=1;
    for i=2:Nx-1
        Residue=w.*(0.25.*(V(i-1,j)+V(i+1,j)+2*V(i,j-1)+2*g*h+(h^2)*f(i,j))-V(i,j));
        Rmin=Rmin+abs(Residue);
        V(i,j)=V(i,j)+Residue;
    end
    for j=2:Ny-1
        for i=2:Nx-1
            Residue=w.*(0.25.*(V(i-1,j)+V(i+1,j)+V(i,j-1)+V(i,j+1)+(h^2)*f(i,j))-V(i,j));
            Rmin=Rmin+abs(Residue);
            V(i,j)=V(i,j)+Residue;
        end
    end
end
end

```

Handwritten notes:

- V (with a diagram of a rectangular grid)
- $V_{i,j} = \frac{1}{4}(V_{i-1,j} + V_{i+1,j} + V_{i,j-1} + V_{i,j+1}) + g h + \frac{h^2}{4} f(i,j)$
- $w = \cos(\pi/Nx)$
- $V_{i,j} = \frac{1}{4}(V_{i-1,j} + V_{i+1,j} + V_{i,j-1} + V_{i,j+1}) + g h + \frac{h^2}{4} f(i,j)$

```

j=Ny;
for i=2:Nx-1
    Residue=w.*(0.25.*(V(i-1,j)+V(i+1,j)+2*V(i,j-1)+2*g*h+(h^2)*f(i,j))-V(i,j));
    Rmin=Rmin+abs(Residue);
    V(i,j)=V(i,j)+Residue;
end
Rmin=Rmin/(Nx*Ny); % Average Residue per grid point
if(Rmin>=0.00001) 10^-5
    Ncount=Ncount+1;
    if(Ncount>M)
        loop=0;
        disp(['solution doesnt converge in ',num2str(M),' iter'])
    end
else
    loop=0;
    disp(['solution converges in ',num2str(Ncount),' iteration'])
end
end

```

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

PROBLEM-4

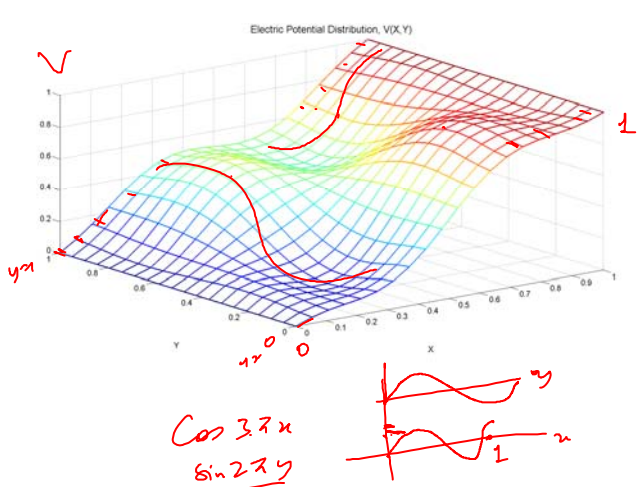
```

% Plot the result
X=xa:dx:xb;%1:Nx;
Y=ya:dy:yb;%1:Ny;
mesh(X,Y,V','linewidth',2);
h=gca;
get(h,'FontSize');
set(h,'FontSize',16);
%colorbar('location','eastoutside','fontsize',12);
%axis([1 Nx 1 Ny])
xlabel('X','fontSize',16);
ylabel('Y','fontSize',16);
title('Electric Potential Distribution, V(X,Y)','fontSize',20);
fh = figure(1);
set(fh, 'color', 'white');

```

Handwritten notes:

- V
- X, Y
- $Y \approx 0$
- $\cos 3.7x$
- $\sin 2.7y$



SEMICONDUCTOR DEVICE MODELING AND SIMULATION

