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Computational Electronics

Solution Details

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Solution of the Coupled DD Equations

There are two schemes that are used in solving the coupled set of equations which comprises the Drift-Diffusion model:

- Gummel's method
- Newton's method

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Gummel’s Method

(A) Gummel’s Relaxation Method

Gummel’s relaxation method, which solves the equations with the decoupled procedure, is used in the case of weak coupling:

- Low current densities (leakage currents, subthreshold regime), where the concentration dependent diffusion term in the current continuity equation is dominant
- The electric field strength is lower than the avalanche threshold, so that the generation term is independent of ∇V
- The mobility is nearly independent of ***E***

The computational cost of the Gummel’s iteration is one matrix solution for each carrier type plus one iterative solution for the linearization of the Poisson Equation

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Gummel’s Method, Cont’d

The solution strategy when using Gummel’s relaxation scheme is the following one:

- Find the equilibrium solution of the linearized Poisson equation

$$\frac{d^2\delta\overline{V}}{d\overline{x}^2}-\frac{n_i}{N}[\mathbf{exp}(\overline{V})+\mathbf{exp}(-\overline{V})]\delta\overline{V}=$$
$$-\frac{d^2\overline{V}}{d\overline{x}^2}+\frac{n_i}{N}\left[\mathbf{exp}(\overline{V})-\mathbf{exp}(-\overline{V})+\frac{N_A-N_D}{n_i}\right]$$

- After the solution in equilibrium is obtained, the applied voltage is increased in steps $\Delta V \leq V_T$
- Now the scaled Poisson equation becomes:

$$\frac{d^2\overline{V}}{d\overline{x}^2}=\frac{n_i}{N}\left[\mathbf{exp(}-\overline{\phi}_n\mathbf{)}\,\mathbf{exp}(\overline{V})-\mathbf{exp(}\overline{\phi}_p\mathbf{)}\,\mathbf{exp}(-\overline{V})+\frac{N_A-N_D}{n_i}\right]$$

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Gummel's Method, Cont'd

The 1D discretized electron current continuity equation (as long as Einstein's relations are valid) is:

$$\frac{D_{i+1/2}}{a_i}\left[n_{i+1}B(\overline{V}_{i+1}-\overline{V}_i)-n_iB(\overline{V}_i-\overline{V}_{i+1})\right]$$

$$+\frac{D_{i-1/2}}{a_i-1}\left[n_{i-1}B(\overline{V}_{i-1}-\overline{V}_i)-n_iB(\overline{V}_i-\overline{V}_{i-1})\right]+\frac{1}{2}(a_{i-1}+a_i)(G-R)_i=0$$

For holes, one can obtain analogous equations by substituting: $V \to -V, \quad n \to p$

The *decoupled* iteration scheme goes as follows:

(1) Solve the Poisson equation with a guess for the quasi-Fermi levels (use the applied voltage as initial guess)

(2) The potential is used to update the Bernouli functions

(3) The above equations are solved to provide an update for the quasi-Fermi levels, that enter into the Poisson equation

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Gummel's Method, Cont'd

The criterion for convergence is:

$$\mathbf{max}\left|V^{k+1}-V^k\right|, \quad \mathbf{max}\left|V_T\,\mathbf{ln}\left(\frac{n^k}{n^{k+1}}\right)\right|, \quad \mathbf{max}\left|V_T\,\mathbf{ln}\left(\frac{p^k}{p^{k+1}}\right)\right|$$

In the case of strong coupling, one can use the extended Gummel's scheme

$$V^{k+1}=V^k+\delta V$$

$$n^{k+1}=n^k\,\mathbf{exp}\left[\frac{\delta V}{V_T}\right]\left(1-\delta V+V_T\,\mathbf{ln}\left[\frac{\delta n}{n^k}\right]\right)$$

$$p^{k+1}=p^k\,\mathbf{exp}\left[\frac{\delta V}{V_T}\right]\left(1-\delta V+V_T\,\mathbf{ln}\left[\frac{\delta p}{p^k}\right]\right)$$

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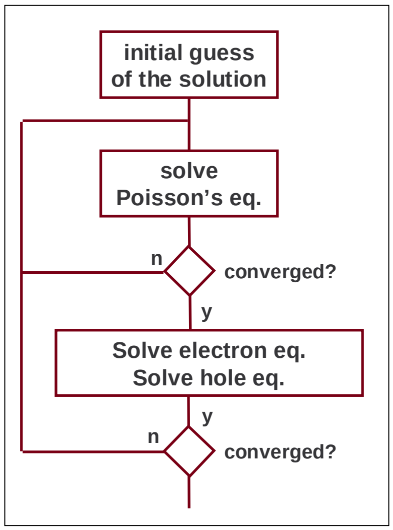
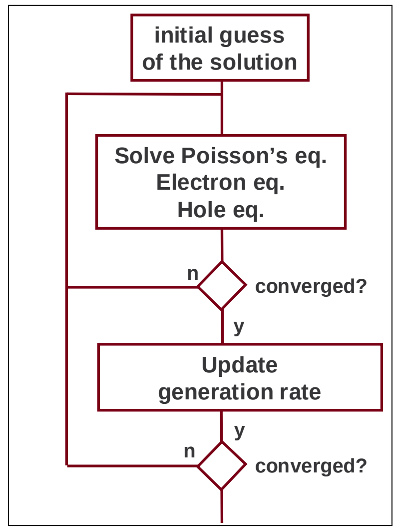
Gummel's Method, Cont'd

Original Gummel's scheme



Modified Gummel's scheme



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Newton's Method

(B) Newton's method

- The three equations that constitute the DD model, written in residual form are:

$$F_V(v,n,p)=0 \qquad F_n(v,n,p)=0 \qquad F_p(v,n,p)=0$$

- Starting from an initial guess, the corrections are calculated by solving:

$$\begin{bmatrix} \frac{\partial F_V}{\partial v} & \frac{\partial F_V}{\partial n} & \frac{\partial F_V}{\partial p} \\ \frac{\partial F_n}{\partial v} & \frac{\partial F_n}{\partial n} & \frac{\partial F_n}{\partial p} \\ \frac{\partial F_p}{\partial v} & \frac{\partial F_p}{\partial n} & \frac{\partial F_p}{\partial p} \end{bmatrix} \cdot \begin{bmatrix} \Delta v \\ \Delta n \\ \Delta p \end{bmatrix} = \begin{bmatrix} F_V \\ F_n \\ F_p \end{bmatrix} \Rightarrow \begin{matrix} V^{k+1} = V^k + \Delta V^k \\ n^{k+1} = n^k + \Delta n^k \\ p^{k+1} = p^k + \Delta p^k \end{matrix}$$

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Newton's Method, Cont'd

- The method can be simplified by the following iterative scheme:

$$\begin{bmatrix} \frac{\partial F_V}{\partial V} & 0 & 0 \\ \frac{\partial F_n}{\partial V} & \frac{\partial F_n}{\partial n} & 0 \\ \frac{\partial F_p}{\partial V} & \frac{\partial F_p}{\partial n} & \frac{\partial F_p}{\partial p} \end{bmatrix} \cdot \underset{k+1}{\begin{bmatrix} \Delta V \\ \Delta n \\ \Delta p \end{bmatrix}} = -\begin{bmatrix} F_V \\ F_n \\ F_p \end{bmatrix} - \begin{bmatrix} 0 & \frac{\partial F_V}{\partial n} & \frac{\partial F_V}{\partial p} \\ 0 & 0 & \frac{\partial F_n}{\partial n} \\ 0 & 0 & 0 \end{bmatrix} \cdot \underset{k}{\begin{bmatrix} \Delta V \\ \Delta n \\ \Delta p \end{bmatrix}}$$

$$\frac{\partial F_V}{\partial V}\Delta V^{k+1} = -F_V - \frac{\partial F_V}{\partial n}\Delta n^k - \frac{\partial F_V}{\partial p}\Delta p^k$$

$$\frac{\partial F_V}{\partial V}\Delta n^{k+1} = -F_n - \frac{\partial F_n}{\partial V}\Delta V^{k+1} - \frac{\partial Fn}{\partial p}\Delta p^k$$

$$\frac{\partial F_p}{\partial p}\Delta p^{k+1} = -F_p - \frac{\partial F_p}{\partial V}\Delta V^{k+1} - \frac{\partial F_p}{\partial n}\Delta n^{k+1}$$

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Carrier Action

- Drift process
- Diffusion process
- Generation-recombination mechanisms

Drift Process

Drift process:

- Under low-field conditions, the carrier drift velocity is proportional to the electric field:

  $\mathbf{v}_{dn}=-\mu_n\mathbf{F}$ (for electrons) and $\mathbf{v}_{dp}=\mu_p\mathbf{F}$ (for holes)

- These expressions can be obtained from the second law of motion. For example, for an electron moving in an electric field, one has:

$$m_n^* \frac{d\mathbf{v}_{dn}}{dt} = -q\mathbf{F} - m_n^* \frac{\mathbf{v}_{dn}}{\tau_m}$$

- Low frequency limit:

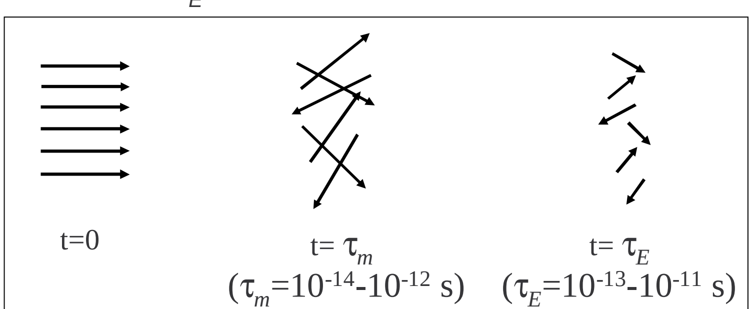
$$-q\mathbf{F} - m_n^* \frac{\mathbf{v}_{dn}}{\tau_m} = 0 \rightarrow \mathbf{v}_{dn} = -\frac{q\tau_m}{m_n^*}\mathbf{F} = -\mu_n \mathbf{F} \rightarrow \mu_n = \frac{q\tau_m}{m_n^*}$$

Drift Process, …

- The linear dependence of **v** on **F** does not hold at high fields when electrons gain considerable energy from the electric field, in which case one has:

$$\frac{dE}{dt} = q\mathbf{v}\cdot\mathbf{F} - \frac{E-E_0}{\tau_E} \xrightarrow{\text{steady-state}} E = E_0 + q\tau_E \mathbf{v}\cdot\mathbf{F}$$

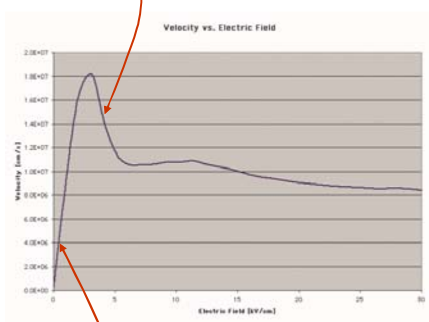
- Description of the momentum relaxation time τ_m and energy relaxation time τ_E:



Drift Process, …

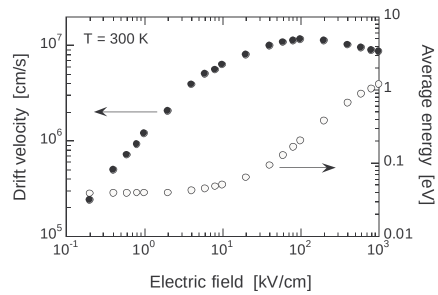
- Drift velocity for GaAs and Si:

Intervalley transfer



Slope $dv_d/dF=\mu$

GaAs

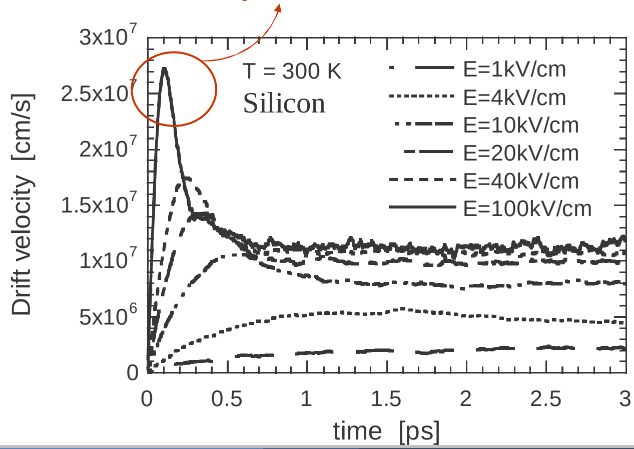


Silicon

Drift Process, …

- Small devices => non-stationary transport
  velocity overshoot => faster devices (smaller transit time)

Velocity overshoot effect



Carrier Mobility:

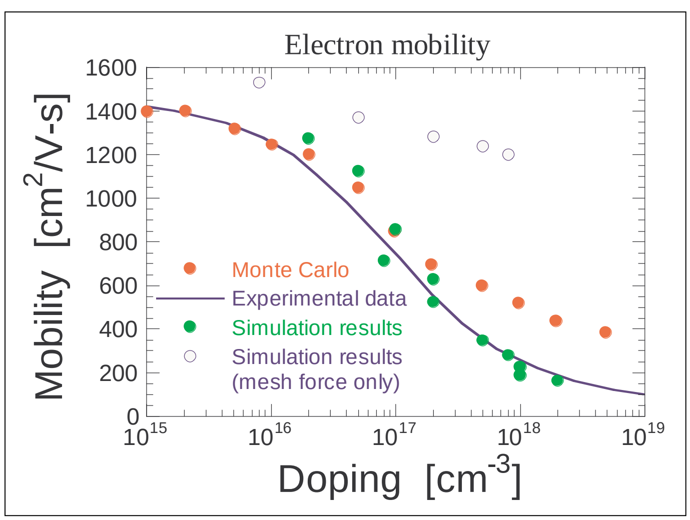
$$\frac{1}{\tau_m} = \frac{1}{\tau_{ii}} + \frac{1}{\tau_{ni}} + \frac{1}{\tau_{ac}} + \frac{1}{\tau_{npo}} + \frac{1}{\tau_{po}} + \frac{1}{\tau_{pe}}$$

- τ_{ii}: Ionized impurities Si, GaAs
- τ_{ni}: neutral impurities (low T) Si, GaAs
- τ_{ac}: Acoustic phonons Si, GaAs
- τ_{npo}: Non-polar optical phonons Si
- τ_{po}: polar optical phonons GaAs
- τ_{pe}: Piezoelectric (low-T) GaAs

Mathiessen's rule:

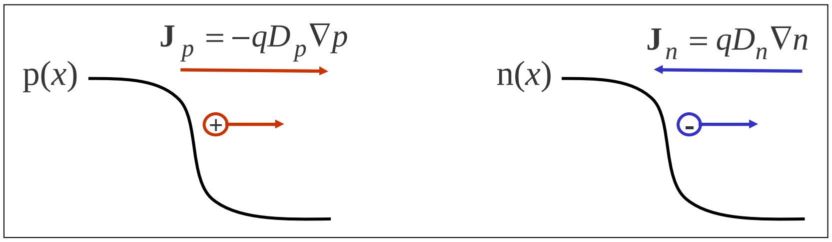
$$\frac{1}{\mu} = \frac{1}{\mu_{ii}} + \frac{1}{\mu_{ni}} + \frac{1}{\mu_{ac}} + \frac{1}{\mu_{npo}} + \frac{1}{\mu_{po}} + \frac{1}{\mu_{pe}} \Rightarrow \begin{array}{l} \mu_l \propto T^{-3/2} \\ \mu_{ii} \propto T^{3/2} N_I^{-1} \\ \mu_{ni} \propto N_0^{-1} \end{array}$$

Carrier Mobility (Cont'd):



Diffusion Process

Diffusion process:



- ***D_n, D_p*** ➔ **Diffusion** constants for electrons and holes
- **Total current** equals the sum of the drift and diffusion components:

$$\mathbf{J}_n = qn\mu_n \mathbf{F} + qD_n \nabla n$$

$$\mathbf{J}_p = qp\mu_p \mathbf{F} - qD_p \nabla p$$

Diffusion Process, ...

Einstein relations (derivation):

Assumptions:

- equilibrium conditions
- non-degenerate semiconductor

$$J_n = qn\mu_n F + qD_n \frac{\partial n}{\partial x} = 0$$

$$n = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right) \quad \rightarrow \quad n = n_i \exp\left(\frac{E_F - E_i}{k_B T}\right)$$

$$\frac{\partial n}{\partial x} = \left(\frac{\partial E_F}{\partial x} - \frac{\partial E_i}{\partial x}\right)\frac{1}{k_B T} n_i \exp\left(\frac{E_F - E_i}{k_B T}\right) \rightarrow \frac{\partial n}{\partial x} = -\frac{q}{k_B T} nF$$

$$\downarrow qn\mu_n F + qD_n\left(-\frac{q}{k_B T}\right)nF = 0 \rightarrow \begin{cases} D_n / \mu_n = k_B T / q = V_T \\ D_p / \mu_p = k_B T / q = V_T \end{cases}$$

Generation-Recombination Mechanisms:

Photons and phonons (review)

- **Photons** ➔ quantum of energy in an electromagnetic wave

$$E = hf \approx (1-4)\,eV$$
$$p = h/\lambda, \quad \lambda = c/f \approx 0.4\mu m \;\; (E = 1eV)$$
$$\downarrow$$
large energy, small momentum

- **Phonons** ➔ quantum of energy in an elastic wave

$$E = hf \approx (0.02 - 0.06)\,eV$$
$$p = h/\lambda, \quad \lambda = v_s/f \approx 1.8nm$$
$$(E = 0.02eV, v_s = 8.5\times 10^3 m/s)$$
$$\downarrow$$
small energy, large momentum

Notation:

g ➔ generation rate
r ➔ recombination rate
R = r - g ➔ net recombination rate

Importance:

BJTs ➔ R plays a crucial role in the operation of the device

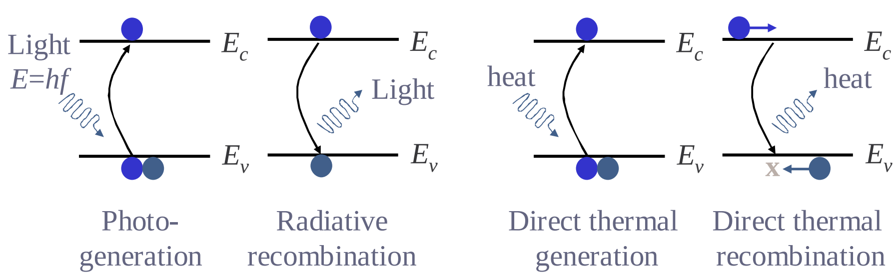
Unipolar devices (MOSFET's, MESFETs, Schottky diodes ➔ No influence except when investigating high-field and breakdown phenomena

Classification

- **Two particle** → Energy-level consideration
  - One step (Direct) →
    - Photogeneration
    - Radiative recombination
    - Direct thermal generation
    - Direct thermal recomb.
  - Two-step (indirect) →
    - Shockley-Read-Hall (SRH) generation-recombination
    - Surface generation-recombination
- **Three particle** →
  - Impact ionization → Pure generation process
  - Auger →
    - Electron emission
    - Hole emission
    - Electron capture
    - Hole capture

(1) Direct Processes

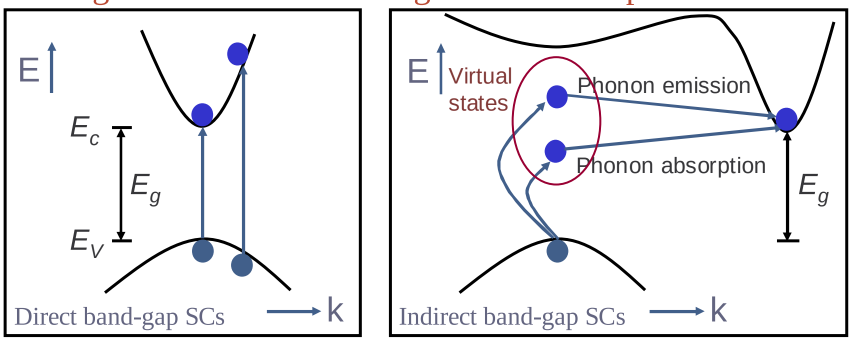
Diagramatic description:



Important for:
- narrow-gap semiconductors
- direct band-gap SCs used for fabricating LEDs for optical communications

Not the usual means by which the carriers are generated or recombine

- Photogeneration ➔ band-diagramatic description:



Momentum and energy conservation:

$$p_f = p_i$$
$$E_f = E_i + E_{ph}$$

final initial photon

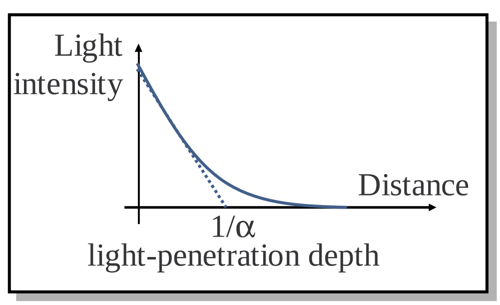
$$p_f = p_i \mp p_s$$
$$E_f = E_i \mp E_s + E_{ph}$$

final initial phonon

Near the absorption edge, the absorption coefficient can be expressed as:

$$\alpha \propto \left(hf - E_g\right)^{\gamma}$$

hf = photon energy
$\boldsymbol{E_g}$ = bandgap



γ = constant

➔ γ = 1/2 and 1/3 for allowed direct transitions and forbidden direct transitions

➔ γ = 2 for indirect transitions where phonons are involved

- Photogeneration-radiative recombination ➔ mathematical description

  - Both types of carriers are involved in the process:

$$r = Bpn, \quad g = Bp_0 n_0 = Bn_i^2$$

$$R = r - g = B\left(pn - n_i^2\right) \rightarrow p = p_0 + \Delta p, \; n = n_0 + \Delta n$$

$$R = B \cdot \Delta n\left(p_0 + n_0 + \Delta n\right)$$

$$\begin{cases} B(GaAs) = (1.3 \pm 0.3) \times 10^{-10}\, cm^3/s \\ B(Si) = 2 \times 10^{-15}\, cm^3/s \end{cases}$$

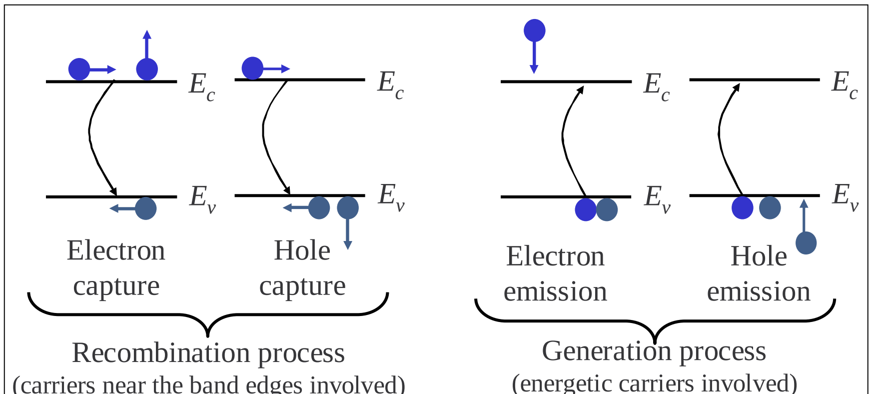
  - Limiting cases:

    (a) Low-level injection: $\Delta n, n_0 << p_0 \rightarrow \tau_{rad} = \dfrac{\Delta n}{R} \approx \dfrac{1}{Bp_0}$

    (b) High-level injection: $\Delta n >> n_0, p_0 \rightarrow \tau_{rad} = \dfrac{\Delta n}{R} \approx \dfrac{1}{B\Delta n}$

(2) Auger Process

Diagramatic description:



- Auger generation takes place in regions with high concentration of mobile carriers with negligible current flow
- Impact ionization requires non-negligible current flow

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- **Auger process ➔ mathematical description**
  - Three carriers are involved in the process

$$r = C_n p n^2 + C_p p^2 n, \quad g = C_n p_0 n_0^2 + C_p p_0^2 n_0$$
$$R = r - g = C_n\left(pn^2 - p_0 n_0^2\right) + C_p\left(p^2 n - p_0^2 n_0\right)$$
$$\downarrow$$
$$p = p_0 + \Delta p, \; n = n_0 + \Delta n$$
$$\tau_{Auger} = \frac{\Delta n}{R} = \frac{1}{aC_p + bC_n} \rightarrow \begin{cases} a = p_0^2 + 2n_0 p_0 + \Delta n(2p_0 + n_0 + \Delta n) \\ b = n_0^2 + 2n_0 p_0 + \Delta n(2n_0 + p_0 + \Delta n) \end{cases}$$

  - Limiting cases (*p*-type sample):

(a) Low-level injection: $\tau_{Auger} = \left[C_p p_0^2 + C_n p_0 (2n_0 + \Delta n)\right]^{-1}$

(b) High-level injection: $\tau_{Auger} = \left[\Delta n^2 \left(C_p + C_n\right)\right]^{-1}$

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(3) Impact Ionization

- Auger Coefficients: (Silvaco)

T [K]	C_n [cm^6/s]	C_p [cm^6/s]
77	2.3×10^{-31}	7.8×10^{-32}
300	2.8×10^{-31}	9.9×10^{-32}
400	2.8×10^{-31}	1.2×10^{-31}

<u>(3) Impact ionization:</u>

Diagramatic description ➔ identical to Auger generation

$$G_{impact} = \frac{1}{q}\left[\alpha_n \left|\mathbf{J}_n\right| + \alpha_p \left|\mathbf{J}_p\right|\right]$$

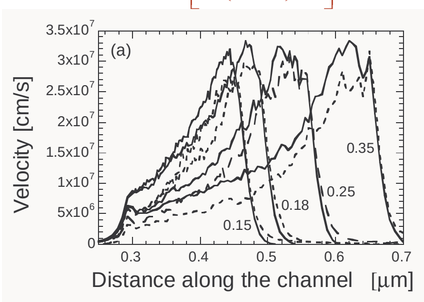
Ionization rates => generated electron hole-pairs per unit length of travel per carrier

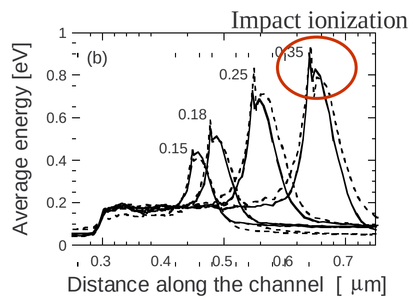
- Ionization rates dependence upon the electric field component parallel to the current flow:

$$\alpha_n = A_n \exp\left[-\left(\frac{E_n^{crit}}{E}\right)^{\beta_n}\right]$$

$$\alpha_p = A_p \exp\left[-\left(\frac{E_p^{crit}}{E}\right)^{\beta_p}\right]$$

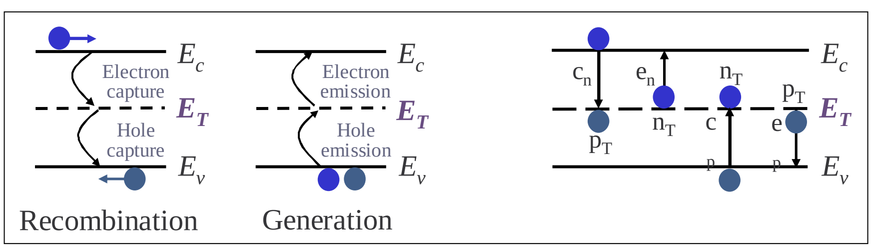
Material	A_n [cm^{-1}]	E_n^{crit} [V/cm]	β_n
Si	1x10^{6}	1.66x10^{6}	1
GaAs	3x10^{5} 2x10^{6}	6.85x10^{5} 2x10^{6}	1.6 1
Ge	1.55x10^{7}	1.56x10^{5}	1





(4) Shockley-Read-Hall Mechanism

Diagramatic description:



Mathematical model:

$$\frac{dn}{dt} = e_n n_T - c_n n p_T$$

$$\frac{dp}{dt} = e_p p_T - c_p p n_T$$

Two types of carriers involved in the process

$$\left.\begin{aligned} n_T &= N_T f_T \\ p_T &= N_T (1 - f_T) \end{aligned}\right\} \rightarrow n_T + p_T = N_T$$

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- Thermal equilibrium conditions:

$$dn/dt = 0,\ dp/dt = 0$$
$$\downarrow$$
$$\begin{cases} c_n n p_T = e_n n_T \\ e_p p_T = c_p p n_T \end{cases} \Rightarrow \begin{cases} e_n = c_n n_1 \\ e_p = c_p p_1 \end{cases}$$

n_1 and p_1 are the electron and hole densities when $E_F = E_T$

- Steady-state conditions:

$$\begin{cases} R_n = R_{nc} - R_{ne} = c_n n p_T - e_n n_T = c_n (n p_T - n_1 n_T) \\ R_p = R_{pc} - R_{pe} = c_p p n_T - e_p p_T = c_p (p n_T - p_1 p_T) \end{cases}$$
$$\Downarrow$$
$$f_T = \frac{c_n n + c_p p_1}{c_n (n + n_1) + c_p (p + p_1)} \rightarrow R = \frac{np - n_i^2}{\frac{1}{c_p N_T}(n + n_1) + \frac{1}{c_n N_T}(p + p_1)}$$

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- Define carrier lifetimes:

$$\tau_p = \frac{1}{c_p N_T} = \frac{1}{\sigma_p v_{th} N_T},\quad \tau_n = \frac{1}{c_n N_T} = \frac{1}{\sigma_n v_{th} N_T}$$

- Empirical expressions for electron and hole lifetimes:

$$\tau_n = \frac{\tau_n^0}{1 + \frac{N_A + N_D}{N_n^{ref}}},\quad \tau_p = \frac{\tau_p^0}{1 + \frac{N_A + N_D}{N_p^{ref}}}$$

τ_{n0} [s]	N_n^{ref} [cm^{-3}]	τ_{p0} [s]	N_p^{ref} [cm^{-3}]	Source
$5\text{x}10^{-5}$	$5\text{x}10^{16}$	$5\text{x}10^{-5}$	$5\text{x}10^{16}$	D'Avanzo
$3.94\text{x}10^{-4}$	$7.1\text{x}10^{15}$	$3.94\text{x}10^{-4}$	$7.1\text{x}10^{15}$	Dhanasekaran

- Limiting cases:

$$\tau_{SRH} = \frac{\Delta n}{R} = \frac{\tau_p(n_0 + \Delta n + n_1) + \tau_n(p_0 + \Delta n + p_1)}{n_0 + p_0 + \Delta n}$$

(a) Low level injection (p-type sample): $\tau_{SRH} = \frac{\Delta n}{R} = \tau_n$

(b) High-level injection: $\tau_{SRH} = \frac{\Delta n}{R} = \tau_n + \tau_p$

- Generation process (p≅n ≅ 0):

$$R = \frac{-n_i^2}{\tau_p n_1 + \tau_n p_1} = -G \rightarrow G = \frac{n_i}{\tau_g}$$

τ_g=generation rate => $\tau_g = \tau_p e^{\alpha} + \tau_n e^{-\alpha}, \quad \alpha = \frac{E_T - E_i}{k_B T}$