

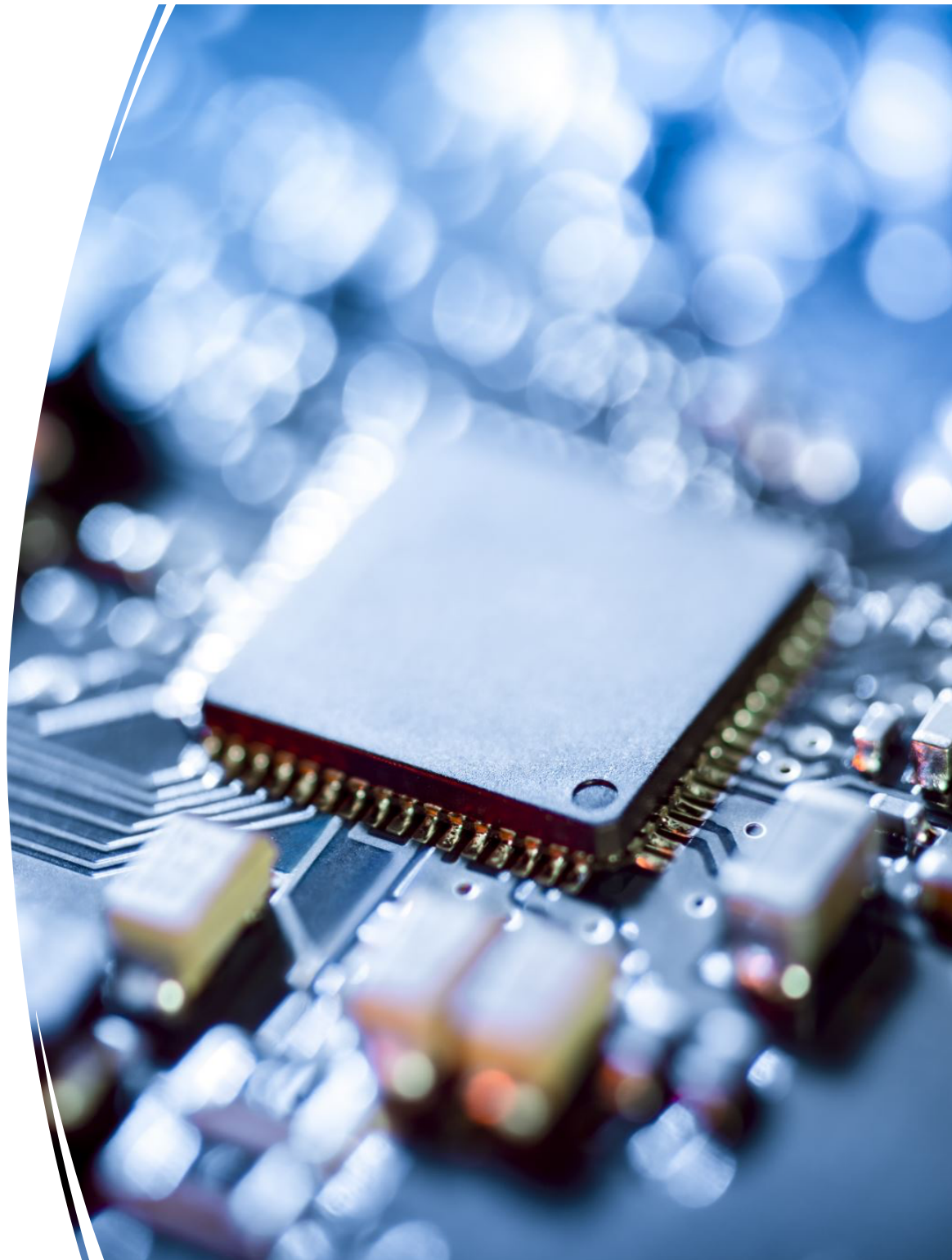
Semiconductor Device Modeling and Simulation

**L4.04 Generation-
Recombination Mechanisms
Modeling**

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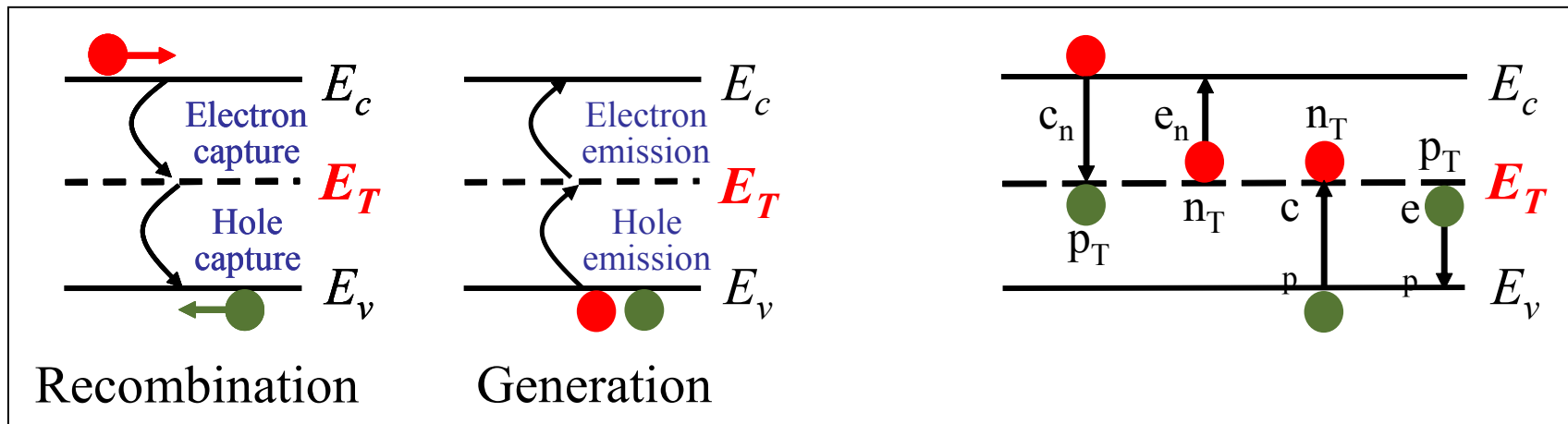
National Nanotechnology
Coordinated Infrastructure



Generation-Recombination Mechanisms

- Shockley-Read-Hall (SRH)
- Radiative Recombination
- Auger Generation-Recombination
- Surface Recombination
- Impact Ionization

Shockley-Read-Hall GR Mechanism



Mathematical formulation and implementation in Silvaco:

$$R_{SRH} = \frac{pn - n_{ie}^2}{\text{TAUP0} \left[n + n_{ie} \exp\left(\frac{\text{ETRAP}}{kT_L}\right) \right] + \text{TAUN0} \left[p + n_{ie} \exp\left(\frac{-\text{ETRAP}}{kT_L}\right) \right]}$$

This model is activated by using the SRH parameter of the MODELS statement. The electron and hole lifetime parameters, TAUN0 and TAUP0, are user-definable in the MATERIAL statement. ETRAP is the difference between the trap level and the intrinsic level.

Shockley-Read-Hall Mechanism

The minority carrier lifetimes are a function of the impurity concentration, and in this case:

$$R_{SRH} = \frac{pn - n_{ie}^2}{\tau_p \left[n + n_{ie} \exp\left(\frac{E_{TRAP}}{kT_L}\right) \right] + \tau_n \left[p + n_{ie} \exp\left(\frac{-E_{TRAP}}{kT_L}\right) \right]}$$

Where:

$$\tau_n = \frac{TAUN0}{AN + BN\left(\frac{Ntotal}{NSRHN}\right) + CN\left(\frac{Ntotal}{NSRHN}\right)^{EN}}$$

$$\tau_p = \frac{TAUP0}{AP + BP\left(\frac{Ntotal}{NSRHP}\right) + CP\left(\frac{Ntotal}{NSRHP}\right)^{EP}}$$

The TAUN0, TAUP0, NSRHN, and NSRHP parameters can be defined on the MATERIAL statement. This model is activated with the CONSRH parameter of the MODELS statement.

Surface Recombination

- Surface recombination process is described with the following way:

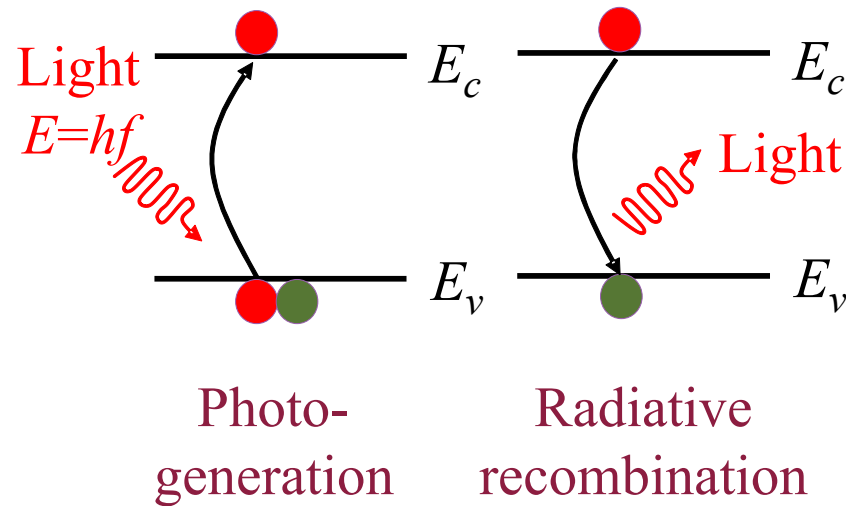
$$R_{surf} = \frac{pn - n_{ie}^2}{\tau_p^{eff} \left[n + n_{ie} \exp\left(\frac{E_{TRAP}}{kT_L}\right) \right] + \tau_n^{eff} \left[p + n_{ie} \exp\left(\frac{-E_{TRAP}}{kT_L}\right) \right]}$$

bulk lifetime

$$\frac{1}{\tau_n^{eff}} = \frac{1}{\tau_n^i} + \frac{d_i}{A_i} S.N \qquad \frac{1}{\tau_p^{eff}} = \frac{1}{\tau_p^i} + \frac{d_i}{A_i} S.P$$

The S.N and S.P parameters are the recombination velocities for electrons and holes respectively, which are user-definable in the INTERFACE statement. This model is activated by the presence of the recombination velocities in the INTERFACE statement.

Radiative Recombination

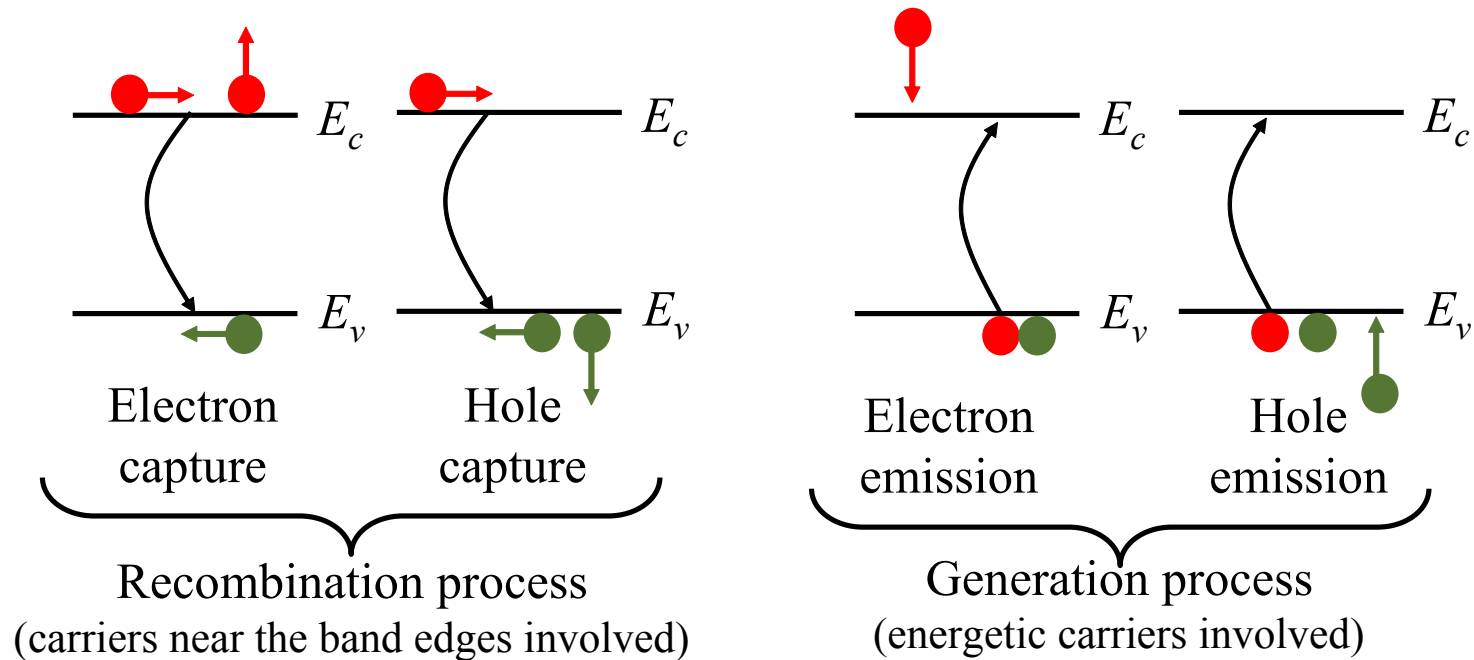


The total band-to-band RG process is given by the following expression:

$$R_{np}^{OPT} = C_c^{OPT} (np - n_{ie}^2)$$

In Atlas, C_c^{OPT} is defined by COPT on the MATERIAL statement. To turn on the optical recombination/generation model, define the OPTR keyword on the MODELS statement.

Auger GR Mechanism



The Auger RG process is given by the following expression:

$$R_{Auger} = AUGN (pn^2 - nn_{ie}^2) + AUGP (np^2 - pn_{ie}^2)$$

The model parameters AUGN and AUGP are user-definable in the MATERIAL statement. You can activate this model with the AUGER parameter from the MODELS statement.

Auger GR Mechanism

In addition to the standard Auger GR Model, there are several other models implemented in Silvaco:

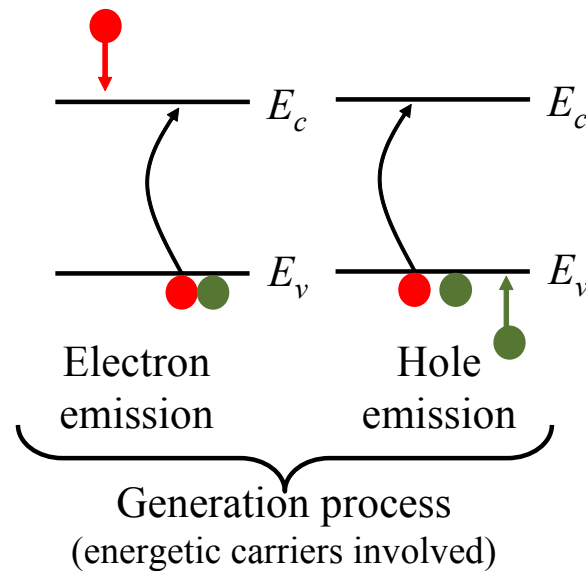
- Klaassen's Temperature-Dependent Auger Model
 - Coefficients C_n and C_p are temperature dependent.
- Narrow Bandgap Auger Model
 - Valid for narrow gap materials for which coefficients C_n and C_p are concentration dependent.
- Auger Recombination Model for High and Low Injection Conditions
 - Coefficients C_n and C_p are carrier and doping concentration dependent.
- Kerr Model for Auger Recombination
 - Applicable to both low and high injection situations.
- Richter Model for Auger Recombination
 - Based on measurements of effective lifetimes of carriers injected into silicon with various doping densities and injection levels. It is an advanced parameterization of the results at 300K that consider Coulomb enhancements.
- Auger Recombination Model With Temperature and Concentration Dependent Coefficients

Impact Ionization Modeling

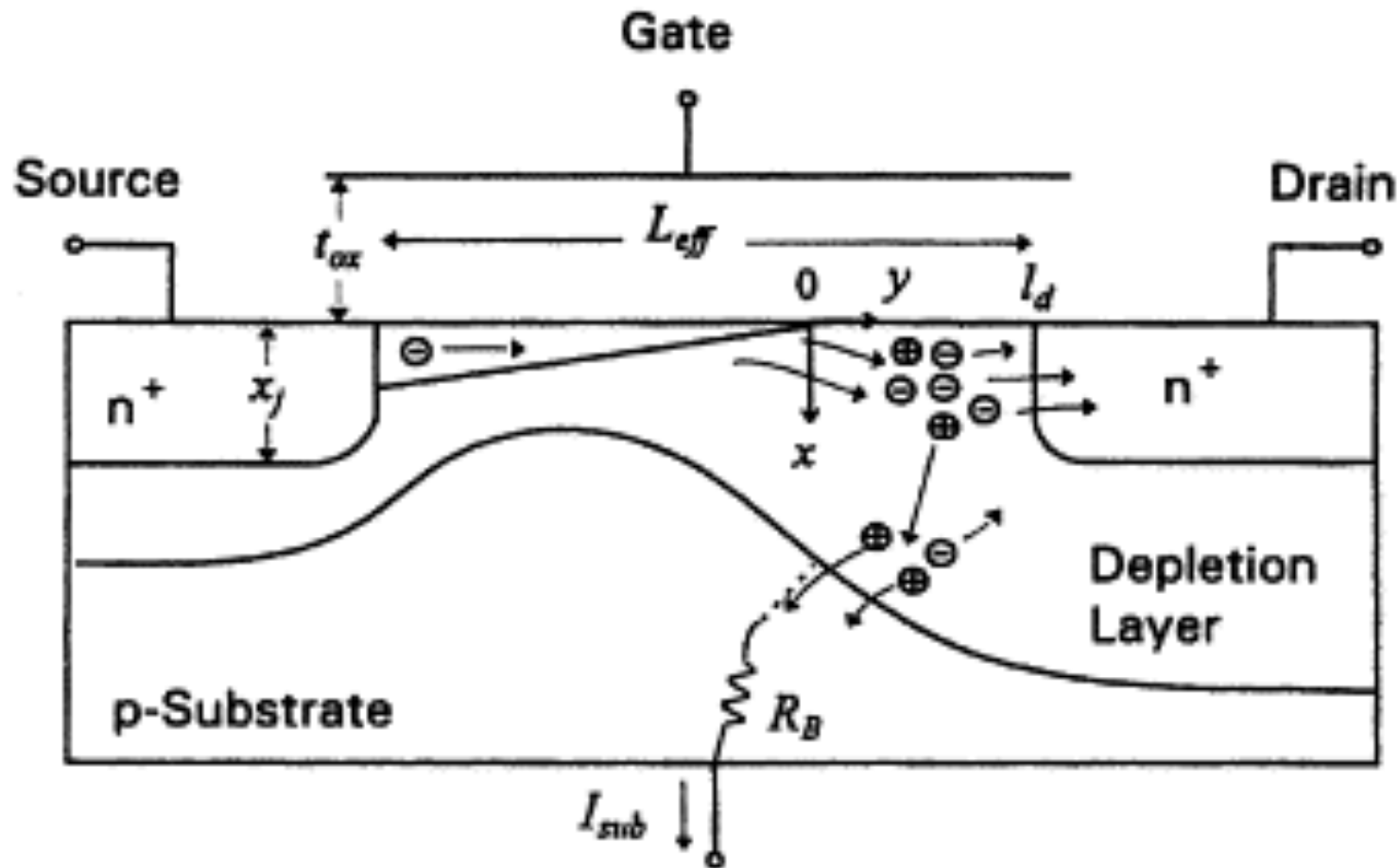
Diagrammatic description → identical to Auger generation

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

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



MOSFET MODELING: Impact Ionization



Silvaco Modeling of Impact Ionization

- The impact ionization models implemented in the Silvaco ATLAS software can be separated into two main categories:



Local impact ionization models:

- Selberherr's model (**SELB** parameter on **IMPACT**)
- Grant's impact ionization model (**GRANT** on the **MODEL** statement)
- Crowell-Sze impact ionization model (**CROWELL** parameter on **IMPACT**)

Non-local models:

- Toyabe ionization model (**TOYABE** parameter on **IMPACT**)
- Concannon's impact ionization model (non-Maxwellian distribution function) (**N.CONCANNON** and **P.CONCANNON** on the **IMPACT** statement)

Selberherr's Model for Impact Ionization

Within the Selberherr's model, the ionization coefficients which appear in the expression for the impact ionization generation rate are calculated using:

$$\alpha_n = \mathbf{AN} \cdot \exp\left[-\left(\frac{\mathbf{BN}}{E}\right)^{\mathbf{BETAN}}\right], \quad \alpha_p = \mathbf{AP} \cdot \exp\left[-\left(\frac{\mathbf{BP}}{E}\right)^{\mathbf{BETAP}}\right]$$

- $\mathbf{AN}, \mathbf{BN}, \mathbf{AP}, \mathbf{BP}$ ➔ temperature-dependent parameters
(specified within the IMPACT statement)
- ➔ can also have different values for electric fields $E < E_{GRAN}$ and $E > E_{GRAN}$

Grant's Impact Ionization Model

Same form as Selberherr's model with two major differences:

- no temperature dependence on **AN, BN, AP, BP** (fixed)
- parameters **AN, BN, AP, BP** have different values for low, intermediate and high electric fields (Baraff)

1) **Low Electric Field** $E < 2.4 \times 10^5 \text{ V/cm}$

$$AN = 2.6 \times 10^6 \quad AP = 2.0 \times 10^6$$

$$BN = 1.43 \times 10^6 \quad BP = 1.97 \times 10^6$$

2) **Intermediate Electric Field** $2.4 \times 10^5 > E > 5.3 \times 10^5 \text{ V/cm}$

$$AN = 6.2 \times 10^5 \quad AP = 2.0 \times 10^6$$

$$BN = 1.08 \times 10^6 \quad BP = 1.97 \times 10^6$$

Parameters are NOT user definable.


3) **High Electric Field** $E > 5.3 \times 10^5 \text{ V/cm}$

$$AN = 5.0 \times 10^5 \quad AP = 5.6 \times 10^5$$

$$BN = 9.9 \times 10^6 \quad BP = 1.32 \times 10^6$$

Crowell-Size Impact Ionization Model

This is a completely different model from the previous two:

$$\alpha_{n,p} = \frac{1}{\lambda_{n,p}} \exp\left[C_0(r) + C_1(r)x + C_2(r)x^2\right]$$


Polynomials in $r = E_r/E_i$

$E_i \Rightarrow$ ionization energy

(1.1 eV for electrons and 1.8 eV for holes)

$E_r = 63 \text{ meV}$

The polynomials $C_i(r)$ and the mean-free path are given by:

$$C_0(r) = -1.92 + 75.5r - 75.7r^2, \quad C_1(r) = -1.75 \times 10^{-2} - 11.9r + 46r^2$$

$$C_2(r) = 3.9 \times 10^{-4} - 1.17r + 11.5r^2$$

$$\lambda_{n,p} = \text{LAMD AE(H)} \frac{\tanh(qE_r / 2k_B T_L)}{\tanh(qE_r / 2k_B 300)}$$

Non-Local Models

- All local electric field-based models will normally **overestimate** the rate of impact ionization.
- This occurs because lucky electron theory inherently assumes that a carrier is traveling through a constant electric field E . As a result, it will predict a distance $\Delta x = E_i / qE$ over which the carrier will gain the ionization energy E_i .
- In real devices, however, the electric field is never constant but is normally sharply peaked at metallurgical junctions. Therefore, as a carrier passes through the peaked electric field the **lucky electron model** will predict the **ionization distance Δx to be too small**. As a result, the ionization rate is **overestimated**.
- The effect of this is that all the simulated breakdown voltages will be **underestimated**, and substrate currents **overestimated**.

Non-Local Models

- The Energy Balance Transport Model can be used to improve the simulation of impact ionization by implementing **ionization models based upon the carrier temperature** instead of the electric field.
- The carrier temperature is a more meaningful basis as the velocity-field relationship is more closely modeled. This allows a non-local dependence on the electric field within the impact ionization model.
- Energy Balance Transport Models will therefore result in more accurate simulations of breakdown voltage and substrate current.
- When the energy balance transport model is applied, only two impact ionization models are available. These are the Toyabe model and the Concannon model.

Toyabe Impact Ionization Model

This is non-local impact ionization model, since the effective electric field that enters into the expression for the calculation of the ionization rate is temperature dependent parameter:

$$\alpha_{n,p} = \mathbf{AN(P)} \cdot \exp\left[-\frac{\mathbf{BN(P)}}{E_{eff,n(p)}}\right], \quad E_{eff,n(p)} = \frac{3}{2q} \frac{k_B T_{n(p)}}{\mathbf{LREL.EL(HO)}}$$

AN, **AP**, **BN**, and **BP** are specified via the **IMPACT** statement

In specifying the relaxation lengths that appear in the above expression, there are two choices:

- Direct specification of **LREL.EL** and **LREL.HO** via the **IMPACT** statement
- Calculate the relaxation lengths using:
LREL.EL = VSATN x TAUSN, **LREL.HO = VSATP x TAUSP**
Where **TAUSN** and **TAUSP** are user specifiable parameters that can be different from **TAUREL.EL** and **TAUREL.HO**

Concannon Impact Ionization Model

Within this model, the generation rates for electrons and holes are calculated using:

$$G_{n,p}(x, y) = \mathbf{CSUB.N(P)} \times n(p) \times \int_{\mathbf{ETH.N(P)}}^{\infty} F[\varepsilon, T_{n,p}(x, y)] d\varepsilon$$

This is where the *non-Maxwellian* distribution function comes into the picture

$$F = \frac{g(\varepsilon) f_{n,p}(\varepsilon)}{\int_0^{\infty} g(\varepsilon) f_{n,p}(\varepsilon) d\varepsilon}$$

where:

$$f_n(\varepsilon) = \left[\exp\left(-\frac{\mathbf{CHIA}\varepsilon^3}{T_n^{1.5}}\right) + \mathbf{C0} \exp\left(-\frac{\mathbf{CHIB}\varepsilon^3}{T_n^{1.5}}\right) \right]$$

$$f_p(\varepsilon) = \exp\left(-\frac{\mathbf{CHI.HOLES}\varepsilon^3}{T_p^{1.5}}\right)$$

All of the above parameters are specified via the IMPACT statement.

Summary

In this lecture we discussed the following generation-recombination mechanisms modeling:

- Shockley-Read-Hall GR mechanism
 - Bulk materials
 - Surfaces/interfaces
- Radiative Recombination
- Auger GR mechanism
- Impact ionization