Genius

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Semiconductor Device Simulator

Version 1.7.4

Genius User's Guide

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CHAPTER 1

PHYSICS IN GENIUS DEVICE SIMULATOR

Since Gummel's original work, the drift-diffusion model has been widely used in the semiconductor device simulation. It is now the de facto industry standard in this field.

The original DD model can be achieved by following approximation from hydrodynamic model:

- Light speed is much faster than carrier speed.
- All the collision is elastic.
- Bandgap does not change during collision.
- Carrier temperature equals to lattice temperature and keeps equilibrium.
- The gradient of driving force should keep small.
- Carrier degenerate can be neglected.

Some improvements have been applied to DD model for extend its capability. These "patches" of course make things complex, but they can deal with real problems.

This chapter describes the DD model and its variations used by GENIUS code for describing semiconductor device behavior as well as physical based parameters such as mobility, recombination rate and son on.

Some improvements have been applied to DD model for extend its capability. These "patches" of course make things complex, but they can deal with real problems.

$$\nabla \cdot \varepsilon \nabla \psi = -q \left(p - n + {N_D}^+ - {N_A}^- \right) \tag{1.1}$$

where, ψ is the electrostatic potential of the vacuum level. This choice makes the description of metal-oxide-semiconductor contact and heterojunction easier. n and p are the electron and hole concentration, ${N_D}^+$ and ${N_A}^-$ are the ionized impurity concentrations. q is the magnitude of the charge of an electron.

The relationship of conduct band E_c, valence band E_v and vacuum level ψ is:

$$E_c = -q\psi - \chi - \Delta E_c \tag{1.2}$$
$$E_v = E_c - E_g + \Delta E_v. \tag{1.3}$$

Level 1 Drift-Diffusion Equation

Level 1 Drift-Diffusion (DDML1) is the fundamental solver of GENIUS code for lattice temperature keeps constant though out the solve procedure.

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Poisson's Equation

$$\nabla \cdot \varepsilon \nabla \psi = -q \left(p - n + {N_D}^+ - {N_A}^- \right) \tag{1.4}$$

where, ψ is the electrostatic potential of the vacuum level. This choice makes the description of metal-oxide-semiconductor contact and heterojunction easier. n and p are the electron and hole concentration, ${N_D}^+$ and ${N_A}^-$ are the ionized impurity concentrations. q is the magnitude of the charge of an electron.

The relationship of conduct band E_c, valence band E_v and vacuum level ψ is:

$$E_c = -q\psi - \chi - \Delta E_c \tag{1.5a}$$
$$E_v = E_c - E_g + \Delta E_v. \tag{1.5b}$$

Here, χ is the electron affinity. E_g is the bandgap of semiconductor. ΔE_c and ΔE_v are the bandgap shift caused by heavy doping or mechanical strain.

Furthermore, the relationship of vacuum level ψ and intrinsic Fermi potential $\psi_{\text{intrinsic}}$ is:

$$\psi = \psi_{\text{intrinsic}} - \frac{\chi}{q} - \frac{E_g}{2q} - \frac{k_b T}{2q} \ln\left(\frac{N_c}{N_v}\right) \tag{1.6}$$

The reference 0eV of energy is set to intrinsic Fermi level of equilibrium state in GENIUS.

Continuity Equations

The continuity equations for electrons and holes are defined as follows:

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla \cdot \vec{J}_n - (U - G) \tag{1.7a}$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla \cdot \vec{J}_p - (U - G) \tag{1.7b}$$

where $\vec{J}_n$ and $\vec{J}_p$ are the electron and hole current densities, U and G are the recombination and generation rates for both electrons and holes.

Drift-Diffusion Current Equations

The current densities $\vec{J}_n$ and $\vec{J}_p$ are expressed in terms of the level 1 drift-diffusion model here.

$$\vec{J}_n = q\mu_n n\vec{E}_n + qD_n\nabla n \tag{1.8a}$$

$$\vec{J}_p = q\mu_p p\vec{E}_p - qD_p\nabla p \tag{1.8b}$$

where μ_n and μ_p are the electron and hole mobilities. $D_n = \frac{k_b T}{q}\mu_n$ and $D_p = \frac{k_b T}{q}\mu_p$ are the electron and hole diffusivities, according to Einstein relationship.

Effective Electrical Field

$\vec{E}_n$and $\vec{E}_p$are the effective driving electrical field to electrons and holes, which related to local band diagram. The band structure of heterojunction has been taken into account here \cite{Lindefelt1994}.

$$\vec{E}_n = \frac{1}{q}\nabla E_c - \frac{k_b T}{q}\nabla\left(\ln(N_c) - \ln(T^{3/2})\right) \tag{1.9a}$$

$$\vec{E}_p = \frac{1}{q}\nabla E_v + \frac{k_b T}{q}\nabla\left(\ln(N_v) - \ln(T^{3/2})\right) \tag{1.9b}$$

The lattice temperature keeps uniform throughout DDML1, the above temperature gradient item takes no effect in fact.

By substituting drift-diffusion model into the current density expressions, and combining with Poisson's equation, the following basic equations for DDML1 are obtained:

$$\frac{\partial n}{\partial t} = \nabla \cdot \left(\mu_n n \vec{E}_n + \mu_n \frac{k_b T}{q} \nabla n \right) - (U - G) \tag{1.10a}$$

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left(\mu_p p \vec{E}_p - \mu_p \frac{k_b T}{q} \nabla p \right) - (U - G) \tag{1.10b}$$

$$\nabla \cdot \varepsilon \nabla \psi = -q(p - n + {N_D}^+ - {N_A}^-) \tag{1.10c}$$

DDML1 is suitable for PN diode, BJT transistor and long gate MOSFET simulation. It is robust, and runs pretty fast for real work. The detailed discretization scheme can be found at [[TODO]].

Level 2 Drift-Diffusion Equation

The Level 2 DD model considers the influence of lattice temperature by solving the extra thermal equation simultaneously with the electrical equations. Also, the formula of drift-diffusion equation should be modified according to \cite{Selberherr1984}.

The electron diffusion current in DDML1 can be written as:

$$\vec{J}_{n,\text{diff}} = \frac{k_b T}{q} \mu_n q \nabla n = k_b T \mu_n \nabla n \tag{1.11}$$

Temperature Gradient Correction

But for DDML2, it has the form of

$$\vec{J}_{n,\text{diff}} = \mu_n k_b (T \nabla n + n \nabla T) \tag{1.12}$$

The hole diffusion current should be modified in the same manner.

$$\vec{J}_{p,\text{diff}} = -\mu_p k_b (T \nabla p + p \nabla T) \tag{1.13}$$

Bandgap Narrowing due to Heavy Doping

When bandgap narrowing effects\label{Bandgap narrowing+Slotboom model} due to heavy doping takes place \cite{Slotboom1977}, the band edge shifts:

$$\Delta E_g = \frac{E_{\text{bgn}}}{2 k_b T} \left[\ln \frac{N_{\text{total}}}{N_{\text{ref}}} + \sqrt{\left(\ln \frac{N_{\text{total}}}{N_{\text{ref}}} \right)^2 + C_{\text{bgn}}} \right]. \tag{1.14}$$

Symbol	Parameter	Unit	Silicon	GaAs
$E_g(300)$	EG300	eV	1.1241	1.424
α	EGALPH	eV/K	2.73×10^{-4}	5.405×10^{-4}
β	EGBETA	K	0	204

Table 1.1: Parameters of the Default band structure model

The intrinsic concentration should be modified:

$$n_{ie} = \sqrt{N_c N_v} \exp\left(-\frac{E_g}{2k_b T}\right) \cdot \exp(\Delta E_g) \tag{1.15}$$

Since the carrier current Equation 1.9,

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involves the energy level of conduction band $N_c$and valence band N_v, the bandgap shift should be attributed to them. The bandgap narrowing is attributed half to the conduction band and another half to the valence band as default:

$$E_c' = E_c - \frac{1}{2}\Delta E_g$$
$$E_v' = E_v + \frac{1}{2}\Delta E_g$$

The parameters used in the default band structure model is listed in Table 1.1,

CHAPTER 2

The Second Chapter Style