Drift-Diffusion Model: Introduction

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The popular drift-diffusion current equations can be easily derived from the Boltzmann transport equation by considering moments of the BTE. Consider steady state conditions and, for simplicity, a 1-D geometry. With the use of a relaxation time approximation, the Boltzmann transport equation may be written [1]

$$\frac{eE}{m^*}\frac{\partial f}{\partial v} + v\frac{\partial f}{\partial x} = \frac{f_0 - f(v,x)}{\tau}.$$

(0.1)

In writing Eq. (3.1) parabolic bands have been assumed for simplicity, and the charge e has to be taken with the proper sign of the particle (positive for holes and negative for electrons). The general definition of current density is repeated here for completeness

$$J(x) = e\int vf(v,x)dv$$

(0.2)

where the integral on the right hand side represents the first 'moment' of the distribution function. This definition of current can be related to Eq. (3.1) after multiplying both sides of (3.1) by v and integrating over v. From the RHS of Eq. (3.1) we get

$$\frac{1}{\tau}\left[\int vf_0 dv - \int vf(v,x)dv\right] = -\frac{J(x)}{e\tau}$$

(0.3)

The equilibrium distribution function is symmetric in v, and hence the first integral is zero. Therefore, we have

$$J(x) = -e\frac{e\tau}{m^*}E\int v\frac{\partial f}{\partial v}dv - e\tau\frac{d}{dx}\int v^2 f(v,x)dv$$

(0.4)

Integrating by parts we have

$$\int v\frac{\partial f}{\partial v}dv = \left[vf(v,x)\right]_{-\infty}^{\infty} - \int f(v,x)dv = -n(x)$$

(0.5)

and we can write

$$\int v^2 f(v, x) dv = n(x) \langle v^2 \rangle \tag{0.6}$$

where $\langle v^2 \rangle$ is the average of the square of the velocity. The drift-diffusion equations are derived

introducing the mobility $\mu = \dfrac{e\tau}{m*}$ and replacing $\langle v^2 \rangle$ with its average equilibrium value $\dfrac{k_B T}{m*}$ for

a 1D case and $\dfrac{3k_B T}{m*}$ for a 3D case, therefore neglecting thermal effects. The diffusion coefficient

D is also introduced, and the resulting drift-diffusion current expressions for electrons and holes

are

$$J_n = qn(x)\mu_n E(x) + qD_n \frac{dn}{dx}$$
$$J_p = qp(x)\mu_p E(x) - qD_p \frac{dn}{dx} \tag{0.7}$$

respectively, where q is used to indicate the absolute value of the electronic charge. Although no direct assumptions on the non-equilibrium distribution function, $f(v,x)$, were made in the derivation of Eqs. (3.7), in effect, the choice of equilibrium (thermal) velocity means that the drift-diffusion equations are only valid for small perturbations of the equilibrium state (low fields). The validity of the drift-diffusion equations is empirically extended by introducing field-dependent mobility $\mu(E)$ and diffusion coefficient $D(\mathbf{E})$, obtained from empirical models or detailed calculation to capture effects such as velocity saturation at high electric fields due to hot carrier effects.

Physical Limitations on Numerical Drift-Diffusion Schemes

The complete drift-diffusion model is based on the following set of equations in 1D:

1.   Current equations

$$J_n = qn(x)\mu_n E(x) + qD_n \frac{dn}{dx}$$
$$J_p = qp(x)\mu_p E(x) - qD_p \frac{dn}{dx} \tag{0.8}$$

2.   Continuity equations

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_n + U_n$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_p + U_p$$

(0.9)

3.   Poisson's equation

$$\nabla \cdot \varepsilon \nabla V = -\left(p - n + N_D^+ - N_A^- \right)$$

(0.10)

where U_n and U_p are the net generation-recombination rates.

The continuity equations are the conservation laws for the charge carriers, which may be easily derived taking the zeroth moment of the time dependent BTE. A numerical scheme which solves the continuity equations should

1. Conserve the total charge inside the device, as well as that entering and leaving.
2. Respect the local positive definite nature of carrier density. Negative density is unphysical.
3. Respect monotonicity of the solution (i.e. it should not introduce spurious space oscillations).

Conservative schemes are usually achieved by subdivision of the computational domain into patches (boxes) surrounding the mesh points. The currents are then defined on the boundaries of these elements, thus enforcing conservation (the current exiting one element side is exactly equal to the current entering the neighboring element through the side in common). For example, on a uniform 2-D grid with mesh size Δ, the electron continuity equation may be discretized in an explicit form as follows [2]

$$\frac{n(i,j;k+1) - n(i,j,k)}{\Delta t} = \frac{J^x(i+\frac{1}{2},j;k) - J^x(i-\frac{1}{2},j;k)}{q\Delta} + \frac{J^y(i,j+\frac{1}{2};k) - J^x(i,j-\frac{1}{2};k)}{q\Delta}$$

(0.11)

In Eq. (3.11), the indices i,j describe spatial discretization, k corresponds to the time progression, and the superscripts x and y denote the x- and y-coordinate of the current density vector. This simple approach has certain practical limitations, but is sufficient to illustrate the idea behind the conservative scheme. With the present convention for positive and negative components, it is easy to see that in the absence of generation-recombination terms, the only contributions to the overall device current arise from the contacts. Remember that, since electrons have negative charge, the particle flux is opposite to the current flux. The actual determination of the current densities appearing in Eq. (3.11) will be discussed later. When the equations are discretized, using finite differences for instance, there are limitations on the choice of mesh size and time step [3]:

1. The mesh size Δx is limited by the Debye length.
2. The time step is limited by the dielectric relaxation time.

A mesh size must be smaller than the Debye length where one has to resolve charge variations in space. A simple example is the carrier redistribution at an interface between two regions with different doping levels. Carriers diffuse into the lower doped region creating excess carrier distribution which at equilibrium decays in space down to the bulk concentration with approximately exponential behavior. The spatial decay constant is the Debye length

$$L_D = \sqrt{\frac{\varepsilon k_B T}{q^2 N}}$$

$$(0.12)$$

where N is the doping density. In GaAs and Si, at room temperature the Debye length is approximately 400 Å when $N \approx 10^{16}\, cm^{-3}$ and decreases to about only 50 Å when $N \approx 10^{18}\, cm^{-3}$.

The dielectric relaxation time is the characteristic time for charge fluctuations to decay under the influence of the field that they produce. The dielectric relaxation time may be estimated using

$$t_{dr} = \frac{\varepsilon}{q N \mu}$$

$$(0.13)$$

To see the importance of respecting the limitations related to the dielectric relaxation time, imagine we have a spatial fluctuation of the carrier concentration, which relaxes to equilibrium according to the rate equation

$$\frac{\partial \Delta n}{\partial t} = -\frac{\Delta n(t=0)}{t_{dr}}$$

(0.14)

A finite difference discretization of this equation gives at the first time step

$$\Delta n\left(\Delta t\right) = \Delta n(0) - \frac{\Delta t \Delta n(0)}{t_{dr}}$$

(0.15)

Clearly, if $\Delta t > t_{dr}$, the value of $\Delta n(\Delta t)$ is negative, which means that the actual concentration is evaluated to be less than the equilibrium value, and it is easy to see that the solution at higher time steps will decay oscillating between positive and negative values of Δn. An excessively large Δt may lead, therefore, to nonphysical results. In the case of high mobility, the dielectric relaxation time can be very small. For instance, a sample of GaAs with a mobility of $6000 cm^2/V-s$ and doping $10^{18} cm^{-3}$ has approximately $t_{dr} \approx 10^{-15} s$, and in a simulation the time step Δt should be chosen to be considerably smaller.

Steady State Solution of Bipolar Semiconductor Equations

The general semiconductor equations for electrons and holes may be rewritten in 3D as

$$\nabla \cdot \left(\varepsilon \nabla V\right) = q\left(n - p + N_B\right)$$
$$\nabla \cdot J_n = qU(n,p) + q\frac{\partial n}{\partial t}$$
$$\nabla \cdot J_p = -qU(n,p) + q\frac{\partial p}{\partial t}$$
$$J_n = q\mu_n\left(-n\nabla V + \frac{k_B T}{q}\nabla n\right)$$
$$J_p = q\mu_p\left(-p\nabla V - \frac{k_B T}{q}\nabla p\right)$$

(0.16)

with $N_B = N_A - N_D$. We note that the above equations are valid in the limit of small deviations from equilibrium, since the Einstein relations have been used for the diffusion coefficient, normally valid for low fields or large devices. The generation-recombination term U will be in general a function of the local electron and hole concentrations, according to possible different physical mechanisms, to be examined later in more detail. We will consider from now on steady state, with the time dependent derivatives set to zero.

These semiconductor equations constitute a coupled nonlinear set. It is not possible, in general, to obtain a solution directly in one step, rather a nonlinear iteration method is required. The two more popular methods for solving the discretized equations are the Gummel's iteration method [4] and the Newton's method [5]. It is very difficult to determine an optimum strategy for the solution, since this will depend on a number of details related to the particular device under study. There are in general three possible choices of variables.

1. Natural variable formulation (V,n,p)

2. Quasi-Fermi level formulation (V,ϕ_n,ϕ_p), where the quasi-Fermi levels derive from the following definition of carrier concentration out of equilibrium (for non-degenerate case)

$$n = n_i \exp\left(\frac{q(V - \phi_n)}{k_B T}\right)$$
$$p = n_i \exp\left(\frac{q(\phi_p - V)}{k_B T}\right)$$

3. Slotboom formulation (V,Φ_n,Φ_p) where the Slotboom [6] variables are defined as

$$\Phi_n = n_i \exp\left(-\frac{q\phi_n}{k_B T}\right)$$
$$\Phi_p = n_i \exp\left(\frac{q\phi_p}{k_B T}\right)$$

The Slotboom variables are, therefore, related to the carrier density expressions, and the extension to degenerate conditions is cumbersome.

Normally, there is a preference for the quasi-Fermi level formulation in steady state simulation, and for the natural variables n and p in transient simulation.

Normalization and Scaling

For the sake of clarity, all formulae have been presented without the use of simplifications or normalization. It is however common practice to perform the actual calculation using normalized units to make the algorithms more efficient, and in cases to avoid numerical overflow and underflow. It is advisable to input the data in M.K.S. or practical units (the use of centimeters is for instance very common in semiconductor practice, instead of meters) and then provide a conversion block before and after the computation blocks to normalize and denormalize the variables. It is advisable to use consistent scaling, rather than set certain constants to arbitrary values. The most common scaling factors for normalization of semiconductor equations are listed in Table 0-1 [7].

Table 0-1. Scaling factors

Variable	Scaling Variable	Formula
Space	Intrinsic Debye length ($N=n_i$)	$L = \sqrt{\dfrac{\varepsilon k_B T}{q^2 N}}$
	Extrinsic Debye length ($N=N_{max}$)	
Potential	Thermal voltage	$V^* = \dfrac{k_B T}{q}$
Carrier concentration	Intrinsic concentration	$N=n_i$
	Maximum doping concentration	$N=N_{max}$
Diffusion coefficient	Practical unit	$D = 1\dfrac{cm^2}{s}$
	Maximum diffusion coefficient	
		$D = D_{max}$
Mobility		$M = \dfrac{D}{V^*}$
Generation-Recombination		$R = \dfrac{DN}{L^2}$

Time

$$T = \frac{L^2}{D}$$

References

1   www.NanoHub.org

2   S. Selberherr, *Simulation of Semiconductor Devices and Processes* (Springer-Verlag, Wien New York).

3   K. Tomizawa, *Numerical Simulation of Submicron Semiconductor Devices* (The Artech House Materials Science Library).

4   H. K. Gummel, "A self-consistent iterative scheme for one-dimensional steady state transistor calculation", *IEEE Transactions on Electron Devices*, Vol. 11, pp.455-465 (1964).

5   T. M. Apostol, Calculus, Vol. II, Multi-Variable Calculus and Linear Algebra (Blaisdell, Waltham, MA, 1969) ch. 1

6   J.W. Slotboom, "Computer-aided two-dimensional analysis of bipolar transistors", *IEEE Transactions on Electron Devices*, Vol. 20, pp. 669-679 (1973).

7   A. DeMari, "An accurate numerical steady state one-dimensional solution of the p-n junction", *Solid-state Electronics*, Vol. 11, pp. 33-59 (1968).