

Non-stationary Device Modeling

Standard device analysis starts from the drift-diffusion equations (continuity, current and Poisson's equations). However, particularly for small devices, these equations do not fully describe the behavior of electrons in semiconductor devices. In particular, hot electron effects are neglected.

The fundamental equation for more detailed device analysis is the Boltzmann Transport Equation (BTE), which can be written

$$\frac{\partial f}{\partial t} = -\vec{v} \cdot \nabla_r f + \frac{q}{\hbar} \mathcal{E} \cdot \nabla_k f + \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} \quad (1)$$

where $f = f(\vec{r}, \vec{k}, t)$ is the density of electrons with wave-vector \vec{k} at spatial location \vec{r} at time t , \vec{v} is the electron group velocity, and \mathcal{E} is the applied electric field. The first term accounts for the movement of electrons in space due to the velocity, the second term accounts for the changes of momentum due to applied forces (only electric field included here) and the third term accounts for collisions with the lattice, which cause scattering and can be written:

$$\left(\frac{\partial f}{\partial t} \right)_{\text{coll}} = \int_{\vec{k}'} \left[S(\vec{r}, \vec{k}', \vec{k}) f(\vec{r}, \vec{k}', t) - S(\vec{r}, \vec{k}, \vec{k}') f(\vec{r}, \vec{k}, t) \right] d\vec{k}' \quad (2)$$

where $S(\vec{r}, \vec{k}, \vec{k}')$ is just the rate of scattering from state \vec{k} to state \vec{k}' .

Equation (1) can be thought of as a continuity equation for the state of the electron population in phase space as well as real space and depends on a number of assumptions:

- Interactions among carriers is weak.
- Band theory and effective mass approximation holds.

- Electric field varies slowly in space (rapid changes due to ion cores, etc. are included in scattering term).
- Only point collisions are considered.
- Electron/electron interaction neglected.
- Scattering probabilities are independent of field.
- The electron gas is not degenerate.
- Effect of magnetic field neglected.

The Boltzmann Transport Equation describes a semi-classical system in which carrier motion results from a series of drifts in response to the electric field interspersed with scattering collisions. The electron motion in between collisions is deterministic and is described by classical mechanics, while the time between collisions and the changes in state due collisions are random processes which depend on the transition rates.

Unfortunately, Equation (1) is an integro-differential equation and is quite difficult to solve. The most widely-used solution technique is the Monte-Carlo method, which is extremely compute-intensive. To have a model which is useful for general device simulation, it is necessary to make some simplifications.

In general, the expected value of any parameter at any spatial location can be obtained by integrating over the states. The electron density is just

$$n = \int_{\vec{k}} f d\vec{k} \quad (3)$$

and the expected value of any other quantity is

$$\langle u \rangle = \frac{1}{n} \int_{\vec{k}} u f d\vec{k} \quad (4)$$

If we simply integrate Equation (1) then over the states,

$$\int_k \frac{\partial f}{\partial t} d\vec{k} = - \int_k \vec{v} \cdot \nabla_r f d\vec{k} + \int_k \frac{q}{\hbar} \mathcal{E} \cdot \nabla_k f d\vec{k} + \int_k \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} d\vec{k} \quad (5)$$

Scattering does not change the number of electrons so the last term is zero. Recombination or impact ionization could be included and in that case the last term would give $G - R$. Derivatives over space and time commute with the phase-space integration and so

$$\frac{\partial}{\partial t} \int_k f d\vec{k} = - \nabla_r \cdot \int_k \vec{v} f d\vec{k} + \frac{q}{\hbar} \mathcal{E} \cdot \int_k \nabla_k f d\vec{k} \quad (6)$$

The integral of the gradient with respect to \vec{k} just depends on the velocity at $+\infty - \infty$ which is zero so

$$\frac{\partial n}{\partial t} = - \nabla_r \cdot (n \langle \vec{v} \rangle) = \frac{1}{q} \nabla_r \cdot J_n \quad (7)$$

the electron continuity equation. It remains to derive the form of $\langle v \rangle$.

For scattering which is either elastic (no energy transfer) or isotropic (random velocity following collision) or for small disturbances from equilibrium,

$$\left(\frac{\partial f}{\partial t} \right)_{\text{coll}} = - \frac{f - f_0}{\tau_m(E)} \quad (8)$$

where f_0 is the equilibrium distribution and $\tau_m(E)$ is the momentum relaxation time as a function of the electron energy.

In steady-state ($\partial f / \partial t = 0$), we can write the distribution function as

$$f = f_0 + \frac{q\tau_m}{\hbar} \mathcal{E} \cdot \nabla_k f - \tau_m \vec{v} \cdot \nabla_r f \quad (9)$$

Since

$$\frac{\nabla_k f}{\hbar} = \frac{\partial f}{\partial E} \frac{\nabla_k E}{\hbar} = \frac{\partial f}{\partial E} \vec{v} \quad (10)$$

If we assume a small electric field and thus a small disturbance in f so that $\partial f/\partial E \cong \partial f_0/\partial E$ and $\nabla_r f \cong \nabla_r f_0$,

$$f = f_0 + \tau_m \vec{v} \cdot \left(\frac{\partial f_0}{\partial E} q \mathcal{E} - \nabla_r f_0 \right). \quad (11)$$

For a uniform system (no concentration gradient), the expression for the current becomes

$$J_n = -\frac{1}{q} n \langle v \rangle = -\frac{1}{q} \left[\int_k \vec{v} f_0 d\vec{k} + \int_k q \tau_m \frac{\partial f_0}{\partial E} \vec{v} (v \cdot \mathcal{E}) d\vec{k} \right] \quad (12)$$

The first term is zero since there is the average velocity is zero in equilibrium. The second term can be integrated by assuming a parabolic band and integrating over $E = m^* \vec{v}^2/2$ just as for the calculation of electron concentration.

$$J_n = \frac{q^2 n \langle \tau_m \rangle}{m^*} \mathcal{E} \quad (13)$$

where

$$\langle \tau_m \rangle = \frac{2 \int_{E_c}^{\infty} \tau_m (-\partial f_0/\partial E) (E - E_c)^{3/2} dE}{3 \int_{E_c}^{\infty} f_0 (E - E_c)^{1/2} dE} \quad (14)$$

and thus the mobility is given by

$$\mu_n = \frac{q \langle \tau_m \rangle}{m^*} \quad (15)$$

Including the spatial dependence and assuming the electron temperature is constant, the current equation becomes

$$J_n = q n \mu_n \mathcal{E} + kT \mu_n \frac{F(\eta)}{dF(\eta)/d\eta} \nabla_r n = q n \mu_n \mathcal{E} + q D_n \nabla_r n \quad (16)$$

The drift diffusion equation relies on the following assumptions.

- Higher order terms are neglected (linear, first order corrections to the distribution function only).

- The partial derivative $(\partial f/\partial t)$ has been neglected, which implies that the time scales over which the fields are changing is large compared to $\langle\tau_m\rangle$.
- Carrier temperature is uniform in time and space. No hot electrons, no lattice temperature gradients.
- The spatial gradient of $\langle\tau_m\rangle$ is neglected.
- Parabolic energy bands.
- Far from boundaries.

For small devices, in which hot electron effects occur, many of these assumptions are invalid. To relax these assumptions, we need to include effects due to the deviation of the momentum and energy distribution from the equilibrium distribution f_0 . This can be done by multiplying Equation (1) by higher moments of the velocity ($\vec{p} = m^*\vec{v}$, $E = mv^2/2$) and integrating over k to calculate the time variation of the higher order moments:

$$\frac{dn}{dt} = -\frac{1}{m^*}\nabla \cdot (n\langle\vec{p}\rangle) + G - R \quad (17)$$

$$\frac{d\langle\vec{p}\rangle}{dt} = -\frac{1}{m^*}(\langle p \rangle \cdot \nabla_r)\langle\vec{p}\rangle - q\mathcal{E} - \frac{1}{n}\nabla_r(nkT_e) - \frac{\langle\vec{p}\rangle}{\langle\tau_m\rangle} \quad (18)$$

$$\frac{d\langle E \rangle}{dt} = -\frac{1}{m^*}\langle\vec{p}\rangle \cdot \nabla_r\langle E \rangle - \frac{1}{m^*}q\mathcal{E} \cdot \langle\vec{p}\rangle - \frac{1}{nm^*}\nabla_r \cdot (nkT_e\langle\vec{p}\rangle) - \frac{\langle E \rangle - E_0}{\langle\tau_E\rangle} \quad (19)$$

where the electron temperature is defined by

$$\langle E \rangle = \frac{3}{2}kT_e + \frac{\langle p \rangle^2}{2m^*} \quad (20)$$

These equations are called the hydrodynamic equations and an unlimited number of moments can be calculated. Usually three or four are used with appropriate assumptions made about the higher moments.