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A Study on Steady State Drift-Diffusion Model for Semiconductors

Khin Thi

Abstract

In this paper we discuss the derivation of Drift-Diffusion Model by using Maxwell's equations, Poisson's equation and continuity equations for semiconductors. We also study the existence and uniqueness of solution in steady state.

Key words: continuity; drift-diffusion equation; existence; uniqueness

Introduction

The drift-diffusion equations are the most widely used models to describe semiconductor devices today. The interest in the drift-diffusion model is to replace as much laboratory testing as possible by numerical simulation in order to minimize costs. This model may be obtained by taking zeroth order moment of Boltzmann Transport equation and adjoining the Poisson equation.

We shall derive the basic mathematical model for the electrodynamic behaviour of semiconductor devices. A semiconductor device occupies a bounded, simply connected domain in R^3 which we denote by Ω .

Continuity Equations

Applying Maxwell's Equations, we have

$$0 = \text{div } J + \frac{\partial e}{\partial t}. \quad (1)$$

We split the conduction current density J into electron current density J_n and hole current density J_p :

$$J = J_n + J_p. \quad (2)$$

For the following we assume that the doping profile is time-

invariant:
$$\frac{\partial C}{\partial t} = 0. \quad (3)$$

By using equations Maxwell's and Poisson's Equations, we have:

$$-divJ_p - q \frac{\partial p}{\partial t} = divJ_n - q \frac{\partial n}{\partial t}, \quad x \in \Omega. \quad (4)$$

We obtain equations for the electron and hole current density by setting both sides of (4) equal to a quantity, which we write as qR :

$$divJ_n - q \frac{\partial n}{\partial t} = qR, \quad x \in \Omega, \quad (5)$$

$$divJ_p + q \frac{\partial p}{\partial t} = -qR, \quad x \in \Omega. \quad (6)$$

By inspection of the left hand side of Equations (5), (6), the quantity R can be interpreted as the difference of the rate at which electron-hole carrier pairs recombine and the rate at which they are generated in the semiconductor. Therefore we call R the recombination-generation rate.

We identify the two main sources for current flow in semiconductor devices:

(a) diffusion of the electron and hole ensembles with resulting diffusion current densities

$$J_n^{diff}, J_p^{diff},$$

(b) drift of electrons and holes caused by the electric field as deriving force with resulting drift current densities: J_n^{drift}, J_p^{drift} .

The principal assumption to be used is that the electron and hole current flows are determined by linearly superimposing the diffusion and the drift processes, i.e.

$$J_n = J_n^{diff} + J_n^{drift}, \quad J_p = J_p^{diff} + J_p^{drift}. \quad (7)$$

Electrons and holes diffuse from regions of high concentration into regions of low concentration. By Fourier's law, the diffusion flux densities are proportional to the gradients of the corresponding particle concentration. The diffusion current densities are obtained by multiplying the diffusion fluxes with the charge per particle, which is $-q$ for electrons and $+q$ for holes:

$$J_n^{diff} = qD_n \text{ grad } n \quad (8)$$

$$J_p^{diff} = -qD_p \text{grad } p \quad (9)$$

The signs of the right hand sides are chosen such that the diffusion coefficients D_n and D_p are positive. The electric field driven drift current densities are defined as the products of the charge per particle, the corresponding carrier concentration and the average drift velocity, denoted by v_n^d for electron and v_p^d for holes:

$$J_n^{drift} = -qnv_n^d \quad (10)$$

$$J_p^{drift} = qnv_p^d \quad (11)$$

The drift direction of the carriers are assumed to be parallel to the electric field, the drift of holes has the same orientation as the electric field, while the drift of electrons has opposite orientation. The drift velocities are proportional to the electric field at moderate field strengths

$$v_n^d = -\mu_n E, \quad v_p^d = \mu_p E, \quad (12)$$

where the positive coefficients μ_n , μ_p are called electron and hole mobility respectively.

By inserting Equation (12) into Equations (10-11) and by using (7-9) we obtain the current relations:

$$J_n = qD_n \text{grad } n + q\mu_n nE, \quad x \in \Omega \quad (13)$$

$$J_p = -qD_p \text{grad } p + q\mu_p pE, \quad x \in \Omega. \quad (14)$$

Usually, the diffusion coefficients D_n and D_p are related to the mobilities μ_n , μ_p by Einstein's relations:

$$D_n = U_T \mu_n, \quad D_p = U_T \mu_p$$

where U_T stands for the thermal voltage given by

$$U_T = \frac{k_B T}{q}. \quad k_B \text{ denotes Boltzmann's constant and } T \text{ the device temperature.}$$

Existence and Uniqueness of the Stationary Drift-Diffusion Equations

We consider the system of partial differential equations

$$(a) \quad \text{div}(\varepsilon \text{grad } V) = q(n - p - C)$$

$$\begin{aligned}
 \text{(b)} \quad & \text{div} J_n = q(\partial_t n + R) \\
 \text{(c)} \quad & \text{div} J_p = q(-\partial_t p - R) \\
 \text{(d)} \quad & J_n = q(D_n \text{grad } n - \mu_n n \text{grad } V) \\
 \text{(e)} \quad & J_p = q(-D_p \text{grad } p - \mu_p p \text{grad } V),
 \end{aligned} \tag{15}$$

where ε is the permittivity constant whose approximate value in silicon is 10^{-12} As V^{-1} cm^{-1} . q is the elementary charge whose value is approximately 10^{-19} As. We assume the device given by a domain $\Omega \subseteq R^d$ with $d = 1, 2$ or 3 . The boundary $\partial\Omega$ of the domain Ω is assumed to consist of a Dirichlet part $\partial\Omega_D$ and a Neumann part $\partial\Omega_N$:

$$\partial\Omega = \partial\Omega_D \cup \partial\Omega_N, \quad \partial\Omega_D \cap \partial\Omega_N = \{ \}. \tag{16}$$

The Dirichlet part $\partial\Omega_D$ of the boundary to Ohmic contacts. There the potential V and the concentrations n and p are prescribed. At Ohmic contacts the space charge, given by the right-hand side of (15)(a) vanishes. So

$$n - p - C = 0 \quad \text{for } x \in \partial\Omega_D \tag{17}$$

holds. Furthermore the system is in thermal equilibrium there, which is expressed by the relation

$$np = n_i^2 \quad \text{for } x \in \partial\Omega_D \tag{18}$$

n_i is the intrinsic density ($\cong 10^{10}$ cm^{-3} in silicon at room temperature).

Moreover, the quasi Fermi levels ϕ_n and ϕ_p , given by

$$\left. \begin{aligned}
 \text{(a)} \quad & \phi_n = V - U_T \ln\left(\frac{n}{n_i}\right), \\
 \text{(b)} \quad & \phi_p = V + U_T \ln\left(\frac{p}{n_i}\right).
 \end{aligned} \right\} \tag{19}$$

Assume the values of the applied voltage at Ohmic contacts. Here U_T denotes the thermal voltage which, at room temperature, is roughly 0.025 V. From the conditions (17)-(19) the boundary value for V , n and p

can be uniquely determined. Inserting (18) into (17) give one quadratic equation for n and p each, which have unique positive solutions given by

$$\left. \begin{aligned} (a) n(x,t) = n_D(x) &= \frac{1}{2}(C(x) + \sqrt{C(x)^2 + 4n_i^2}) \\ (b) p(x,t) = p_D(x) &= \frac{1}{2}(-C(x) + \sqrt{C(x)^2 + 4n_i^2}) \\ &\text{for } x \in \partial\Omega_D \\ (19) \text{ gives the boundary values for the potential } V : \\ (c) V(x,t) = V_D(x,t) &= U(x,t) + V_{bi}(x) \\ V_{bi}(x) &= U_T \text{Ln}\left(\frac{n_D(x)}{n_i}\right) \text{ for } x \in \partial\Omega_D \end{aligned} \right\} \quad (20)$$

$U(x,t)$ denotes the applied potential. We implice that ϕ_n equal ϕ_p at Ohmic contacts. The Neumann parts $\partial\Omega_N$ of the boundary model insulating or artificial surfaces. Thus a zero current flow and a zero electric field in the normal direction are prescribed.

$$\begin{aligned} (a) \frac{\partial V}{\partial \nu}(x,t) &(:= \text{grad } V \cdot \nu) = 0 \\ (b) J_n(x,t) \cdot \nu &= 0, \\ (c) J_p(x,t) \cdot \nu &= 0 \quad \text{for } x \in \partial\Omega_N \end{aligned} \quad (21)$$

Here ν will always denote the unit outward normal vector on the boundary $\partial\Omega$. In addition the concentrations of the free carriers n and p at time $t = 0$ are prescribed.

$$n(x, 0) = n^I(x), \quad p(x, 0) = p^I(x) \quad \text{for } x \in \Omega \quad (22)$$

hold and the complete initial boundary value problem is given by the equations (15), the boundary conditions (20), (21) and the initial conditions (22).

For the recombination rate R in (15) (b) (c) we will only consider the Shockley Read Hall term which is of the form

$$R = \frac{np - n_i^2}{\tau_p(n + n_i) + \tau_n(p + n_i)} \quad (23)$$

Here, again, n_i denotes the intrinsic density. τ_n and τ_p are the lifetimes of electrons and holes respectively.

The drift diffusion Equations (15) are considered at a stationary state and that the time derivatives $\partial_t n$ and $\partial_t p$ are neglected.

We will treat the drift diffusion equations in an unscaled form for the moment. So we consider the system

$$\begin{aligned}
 \text{(a)} \quad & \varepsilon \Delta V = q(n - p - C(x)) \\
 \text{(b)} \quad & \operatorname{div} J_n = qR, \\
 \text{(c)} \quad & J_n = q(D_n \operatorname{grad} n - \mu_n n \operatorname{grad} V) \\
 \text{(d)} \quad & \operatorname{div} J_p = -qR, \\
 \text{(e)} \quad & J_p = q(-D_p \operatorname{grad} p - \mu_p p \operatorname{grad} V).
 \end{aligned} \tag{24}$$

Equation (15) have the disadvantage of containing the convection terms $-n \operatorname{grad} V$ and $-p \operatorname{grad} V$ which prohibit the use of the maximum principle in a simple way. If the Einstein relations

$$D_n = U_T \mu_n, \quad D_p = U_T \mu_p \tag{25}$$

can be assumed, with U_T the thermal voltage, it is beneficial to change from the concentrations n and p to the so called Slotboom variables u and v given by

$$\begin{aligned}
 \text{(a)} \quad & n = n_i e^{\frac{v}{U_T} u} \\
 \text{(b)} \quad & p = n_i e^{-\frac{v}{U_T} v}.
 \end{aligned} \tag{26}$$

The current relations then become

$$\begin{aligned}
 \text{(a)} \quad & J_n = q U_T n_i \mu_n e^{\frac{v}{U_T} u} \operatorname{grad} u, \\
 \text{(b)} \quad & J_p = -q U_T n_i \mu_p e^{-\frac{v}{U_T} v} \operatorname{grad} v.
 \end{aligned} \tag{27}$$

After inserting the current densities J_n and J_p into the continuity Equations (24) (b, d) one obtains the elliptic system

$$\begin{aligned}
 \text{(a)} \quad \varepsilon \Delta V &= qn_i \left(e^{\frac{v}{U_T}} u - e^{\frac{v}{U_T}} v \right) - qC(x) \\
 \text{(b)} \quad U_T n_i \operatorname{div}(\mu_n e^{\frac{v}{U_T}} \operatorname{grad} u) &= R \\
 \text{(c)} \quad U_T n_i \operatorname{div}(\mu_p e^{\frac{v}{U_T}} \operatorname{grad} v) &= R .
 \end{aligned} \tag{28}$$

In this form the continuity Equations (28) (b, c) are self adjoint. In the Slotboom variables u and v the boundary at artificial or insulating surfaces becomes pure Neumann conditions

$$\frac{\partial V}{\partial \nu} \Big|_{\partial \Omega_n} = \frac{\partial u}{\partial \nu} \Big|_{\partial \Omega_n} = \frac{\partial v}{\partial \nu} \Big|_{\partial \Omega_n} = 0. \tag{29}$$

For Ohmic constants we obtain from (28) (a, b, c)

$$V|_{\partial \Omega_D} = V_D|_{\partial \Omega_D}, \quad u|_{\partial \Omega_D} = u_D|_{\partial \Omega_D}, \quad v|_{\partial \Omega_D} = v_D|_{\partial \Omega_D} \tag{30}$$

with $u_D = n_i^{-1} e^{-\frac{v_D}{U_T}} n_D$ and $v_D = n_i^{-1} e^{-\frac{v_D}{U_T}} p_D$. Since n and p represent physical concentrations, the Slotboom variables u and v have to remain positive.

Existence theorems for the Problem (28) – (30) usually employ the Schauder Fixed Point Theorem. The construction of the fixed point map depends on the form of the recombination rate, the mobilities, the geometry and so on. We will use some simplifying assumptions. We will consider the Shockley Read Hall recombination term only. So after changing variables to (V, u, v) the recombination rate R in (28) is of the form

$$R = n_i \frac{uv - 1}{\tau_p \left(e^{\frac{v}{U_T}} u + 1 \right) + \tau_n \left(e^{-\frac{v}{U_T}} v + 1 \right)}. \tag{31}$$

We assume that the mobilities μ_n and μ_p are uniformly bounded functions of positions only and that

$$0 < \underline{\mu}_n \leq \mu_n(x) \leq \bar{\mu}_n, \quad 0 < \underline{\mu}_p \leq \mu_p(x) \leq \bar{\mu}_p, \quad \forall x \in \Omega \tag{32}$$

hold. Furthermore we will take the boundary $\partial \Omega$ and the boundary data ψ_D , u_D , and v_D in (30) to be as smooth as necessary. A condition of the form (32) is necessary, to guarantee the uniform ellipticity of the continuity

equations. Therefore most existence proofs do assume an a priori bound on the mobilities even when modeling them as dependent on the field – grad V . The fixed point map is constructed such that its evaluation only involves the solution of semilinear or linear scalar boundary value problems. Let G be given by $G(u_0, v_0) = (u_1, v_1)$, where (u_1, v_1) is computed from (u_0, v_0) as follows.

Step 1: Solve Poisson's equation

$$-\varepsilon \Delta V + qn_i \left(e^{\frac{v}{U_T}} u_0 - e^{-\frac{v}{U_T}} v_0 \right) - qC(x) = 0$$

$$\left. \frac{\partial V}{\partial \nu} \right|_{\partial \Omega_N} = 0, \quad V|_{\partial \Omega_D} = V_D|_{\partial \Omega_D} \quad (33)$$

for $V = V_1$.

Step 2: Solve

$$(a) \quad -U_T \operatorname{div}(\mu_n e^{\frac{v_1}{U_T}} \operatorname{grad} u) + \frac{uv_0 - 1}{\tau_p \left(e^{\frac{v_1}{U_T}} u_0 + 1 \right) + \tau_n \left(e^{-\frac{v_1}{U_T}} v_0 + 1 \right)} = 0$$

$$(b) \quad \left. \frac{\partial u}{\partial \nu} \right|_{\partial \Omega_N} = 0, \quad u|_{\partial \Omega_D} = u_D|_{\partial \Omega_D} \quad (34)$$

for $u = u_1$.

Step 3: Solve

$$(a) \quad -U_T \operatorname{div}(\mu_n e^{-\frac{v_1}{U_T}} \operatorname{grad} v) + \frac{u_0 v - 1}{\tau_p \left(e^{\frac{v_1}{U_T}} u_0 + 1 \right) + \tau_n \left(e^{-\frac{v_1}{U_T}} v_0 + 1 \right)} = 0.$$

$$(b) \quad \left. \frac{\partial v}{\partial \nu} \right|_{\partial \Omega_N} = 0, \quad v|_{\partial \Omega_D} = v_D|_{\partial \Omega_D} \quad (35)$$

for $v = v_1$.

By solving the boundary value problem (33)-(35), a fixed point of the nonlinear operator G is a weak solution of the coupled problem (28)-(30). The existence of such a fixed point is established by showing that the

map G is completely continuous and by applying the Schauder Fixed Point Theorem.

Of course, for this approach one has to choose an appropriate space for defining G . The map G is well defined; that means that the involved boundary value problems are uniquely solvable. All three problems (33)-(35) can be written in the general form

$$\begin{aligned} -\operatorname{div}(a(x) \operatorname{grad} w) + f(x, w) &= 0, \quad x \in \Omega \\ \frac{\partial w}{\partial \nu} \Big|_{\partial \Omega_N} &= 0, \quad w \Big|_{\partial \Omega_D} = w_D \Big|_{\partial \Omega_D} \end{aligned} \quad (36)$$

where w takes the place of V , u and v respectively. The coefficient $a(x)$ in (36) is either the constant ε or equal to $\mu_n e^{\frac{\psi_1}{\nu_r}}$ or $\mu_p e^{-\frac{\psi_1}{\nu_r}}$.

In any case it is uniformly bounded away from zero if μ_n and μ_p are and if ψ_1 is bounded, which makes the semilinear Equation (36) uniformly elliptic. $f(x, w)$ is monotone increasing function of w in all three cases (33) – (35) if u_0 and v_0 are positive. In (34) and (35) f is linear in w . The existence of a unique solution of semilinear partial differential equations of the type as in (36) is, under certain assumptions, a standard result in the theory of elliptic partial differential equations. The coefficient $a(x)$ in solution $w(x)$ will lie in the intersection of the spaces $L^\infty(\Omega)$ and $H^1(\Omega)$.

$H^1(\Omega)$ is the space of functions which are square integrable and whose gradient is square integrable as well. So $\int_{\Omega} (w(x)^2 + |\nabla w(x)|^2) dx < \infty$ holds.

Lemma:

Let the following assumption hold:

(A₁) The function $f(x, w)$ is monotonically increasing in w for all $x \in \Omega$

(A₂) $a(x) \in L^\infty(\Omega)$ and $a(x) \geq \underline{a} > 0$ holds for some constant \underline{a} .

(A₃) There exist functions $\underline{g}(w)$ and $\tilde{g}(w)$ such that $\underline{g}(w) \leq f(x, w) \leq \tilde{g}(w)$ hold $\forall x \in \Omega, \forall w$.

(A₄) There exist solutions \underline{w} and \tilde{w} of $\underline{g}(\tilde{w}) = 0$ and $\tilde{g}(\underline{w}) = 0$.

Then there exists a unique solution w of the problem (36) in $H^1(\Omega) \cap L^\infty(\Omega)$.

This solution satisfies $\underline{w} \leq w(x) \leq \bar{w}$

$$\underline{w} = \min \left\{ \inf_{\partial\Omega_D} w_D, \underline{w} \right\}, \quad \bar{w} = \max \left\{ \sup_{\partial\Omega_D} w_D, \bar{w} \right\}. \quad (37)$$

By using lemma We can now, by showing that the map G is well defined and completely continuous employ the Schauder theorem to establish the existence of a weak solution to (36)

Theorem. Let $K \geq 1$ be a constant satisfying $\frac{1}{K} \leq u_D(x), v_D(x) \leq K \quad \forall x \in \partial\Omega_D$.

Then the problem

$$(a) \quad \varepsilon \Delta V = qn_i \left(e^{\frac{v}{U_T} u} - e^{\frac{v}{U_T} v} \right) - qC(x)$$

$$(b) \quad U_T n_i \operatorname{div}(\mu_n e^{\frac{v}{U_T}} \operatorname{grad} u) = R$$

$$(c) \quad U_T n_i \operatorname{div}(\mu_p e^{\frac{v}{U_T}} \operatorname{grad} v) = R$$

$$(d) \quad \frac{\partial V}{\partial v} \Big|_{\partial\Omega_N} = \frac{\partial u}{\partial v} \Big|_{\partial\Omega_N} = \frac{\partial v}{\partial v} \Big|_{\partial\Omega_N} = 0$$

$$(e) \quad V|_{\partial\Omega_D} = V_D|_{\partial\Omega_D}, \quad u|_{\partial\Omega_D} = u_D|_{\partial\Omega_D}, \quad v|_{\partial\Omega_D} = v_D|_{\partial\Omega_D}$$

has a solution $(V^*, u^*, v^*) \in (H^1(\Omega) \cap L^\infty(\Omega))^3$ which satisfies the L^∞ -estimate $\frac{1}{K} \leq u(x), v(x) \leq K$ in Ω ,

$$\min \left(\inf_{\partial\Omega_D} V_D, U_T \ln \left[\frac{1}{2Kn_i} (\underline{C} + (\underline{C}^2 + 4n_i^2)^{\frac{1}{2}}) \right] \right) \leq V(x) \quad (38)$$

$$V(x) \leq \max \left(\sup_{\partial\Omega_D} V_D, U_T \ln \left[\frac{K}{2n_i} (\bar{C} + (\bar{C}^2 + 4n_i^2)^{\frac{1}{2}}) \right] \right) \text{ in } \Omega$$

where $C \leq C(x) \leq \bar{C}$ holds.

Proof:

First we choose an appropriate space for the fixed point map G . Let N be defined by

$$N = \{(u, v) \in L^2(\Omega) : \frac{1}{K} \leq u, v \leq K \text{ a.e. in } \Omega\}, \quad (39)$$

where $L^2(\Omega)$ is the space of square integrable functions; i.e., the space of functions (u, v) for which

$$\int_{\Omega} |u(x), v(x)|^2 dx < \infty$$

holds. We show that G maps N into itself and is completely continuous. Given $(u_0, v_0) \in N$, by virtue of Lemma, there exists a solution V_1 of (33). \underline{g} and \tilde{g} can be chosen as

$$\underline{g}(V) = n_i q \left(\frac{1}{K} e^{\frac{v}{U_T}} - K e^{-\frac{v}{U_T}} \right) - q \bar{C} \quad (40)$$

$$\tilde{g}(V) = n_i q \left(K e^{\frac{v}{U_T}} - \frac{1}{K} e^{-\frac{v}{U_T}} \right) - q \underline{C}.$$

Solving $\underline{g}(\tilde{V}) = 0$ and $\tilde{g}(\underline{V}) = 0$ gives

$$\underline{V} = U_T \ln \left[\frac{K}{2n_i} (\bar{C} + (\bar{C}^2 + 4n_i^2)^{\frac{1}{2}}) \right] \quad (41)$$

$$\tilde{V} = U_T \ln \left[\frac{1}{2Kn_i} (\bar{C} + (\bar{C}^2 + 4n_i^2)^{\frac{1}{2}}) \right]$$

Applying Lemma to equation (2.20) we use

$$\tilde{g}(u) = \frac{Ku - 1}{\tau_p \left(\frac{e^{\frac{v}{U_T}}}{K} + 1 \right) + \tau_n \left(\frac{e^{-\frac{v}{U_T}}}{K} + 1 \right)}$$

where $\underline{V} \leq V_1(x) \leq \bar{V}$ holds, and obtain $\underline{u} = \frac{1}{K}$. Analogously we obtain $\bar{u} = K$ which implies

$$\frac{1}{K} \leq u_1(x) \leq K. \quad (42)$$

In the same way we obtain $\frac{1}{K} \leq v_1(x) \leq K$. Thus, G maps N into itself. The continuity of N is a simple consequence of the well posedness of uniformly elliptic boundary value problems. On the other hand the continuous dependence of u_1 and v_1 on the data of the corresponding boundary value problems implies

$$\|u_1\|_{1,2,\Omega} + \|v_1\|_{1,2,\Omega} \leq F(\|u_0\|_{2,\Omega}, \|v_0\|_{2,\Omega}, \|u_D\|_{1,2,\Omega}, \|v_D\|_{1,2,\Omega}) \quad (43)$$

for some positive and continuous function F . Here, the symbols $\|\cdot\|_{2,\Omega}$ and $\|\cdot\|_{1,2,\Omega}$ denote the norms in $L^2(\Omega)$ and $H^1(\Omega)$. So

$$\|f\|_{2,\Omega} = \left(\int_{\Omega} |f(x)|^2 dx \right)^{\frac{1}{2}},$$

$$\|f\|_{1,2,\Omega} = \left(\int_{\Omega} (|f(x)|^2 + |\nabla f(x)|^2) dx \right)^{\frac{1}{2}}$$

holds. Thus $\|u_1\|_{1,2,\Omega} + \|v_1\|_{1,2,\Omega} \leq \text{const}$ holds for all (u_0, v_0) in N . The Rellich Kondrachov Theorem) now assures that $G(N)$ is pre-compact in $(L^2(\Omega))^2$. This, together with the continuity of G , gives complete continuity and the Schauder Fixed Point Theorem assures the existence of a fixed point of G which is a solution of (28)-(30).

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