Free Boundaries in Semiconductor Devices*

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Abstract—The first analyses of semiconductor devices in the 1940s and 50s already considered a splitting of devices into regions of zero space charge and depletion regions. Here it is shown that these simplified models appear as singular limits of the drift-diffusion model for charge transport in semiconductors. The limiting problem for the potential is similar to the so called space charge problem. For *pn*-diodes under certain biasing conditions, an existence result is a by-product of the present analysis.

1. Introduction

A nondimensionalized and simplified version of the classical drift-diffusion model for a steady flow of electrons and holes in a semiconductor is given by the elliptic system

$$\begin{aligned} \lambda^2 \Delta V &= n - p - C, \\ \operatorname{div}(\gamma \nabla n - n \nabla V) &= 0, \\ \operatorname{div}(\gamma \nabla p + p \nabla V) &= 0 \end{aligned} \tag{1}$$

for the unknowns V, n and p denoting the electrostatic potential, the electron density and the hole density, respectively. The equations hold in a domain $\Omega \subset R^3$ representing a *pn*-diode. A *pn*-diode is characterized by the fact that the (given) doping profile $C(\mathbf{x})$, $\mathbf{x} \in \Omega$, is positive in a subdomain Ω_n of Ω and negative in another subdomain Ω_p with $\overline{\Omega}_n \cup \overline{\Omega}_p = \overline{\Omega}$. These subdomains are called n-region and p-region, respectively. The dimensionless parameters

$$\lambda = \frac{1}{L}\sqrt{\frac{\varepsilon U_{bi}}{qC_{max}}}, \quad \gamma = \left(\log \frac{C_{max}}{n_i}\right)^{-1}$$

result from the scaling where the maximal doping concentration C_{max}, the built-in voltage $U_{bi} = U_T/\gamma$ and the device diameter L have been used as reference quantities for densities, the potential and length, respectively. The constants ε, q, n_i and U_T are the permittivity, the elementary charge, the intrinsic density and the thermal voltage, respectively. The scaling is standard (see [5]) with the exception that, to the author's knowledge, the built-in voltage has not been used for the scaling of the potential before.

The boundary of the device consists of two Ohmic contacts, $C_n \subset \partial\Omega \cap \partial\Omega_n$ and $C_p \subset \partial\Omega \cap \partial\Omega_p$, and an insulating part $\partial\Omega_N = \partial\Omega \setminus (C_n \cup C_p)$. At the contacts, the carrier densities satisfy the conditions of zero space charge and thermal equilibrium:

$$n - p - C = 0, \quad np = e^{-2/\gamma}, \qquad \text{on } C_n \cup C_p \tag{2a}$$

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which can be rewritten as Dirichlet conditions for n and p. The contact potential is given by

$$\begin{aligned} V &= U + 1 + \gamma \log \frac{C + \sqrt{C^2 + 4e^{-2/\gamma}}}{2}, \quad \text{on } C_n, \\ V &= -1 - \gamma \log \frac{-C + \sqrt{C^2 + 4e^{-2/\gamma}}}{2}, \quad \text{on } C_p \end{aligned} \tag{2b}$$

where U is the applied voltage. The densities as well as the potential satisfy homogeneous Neumann conditions along the insulating boundary parts. See [5] for more details on the model.

In many practical situations the parameters λ and γ are small compared to one. This motivates considering the limits of (1), (2) as these parameters tend to zero. The limit $\lambda \to 0$ has received considerable attention (see [4] and [5] and the references therein). On the other hand, for voltages of the order of magnitude of λ^{-2}, a limiting problem similar to that for $\gamma \to 0$ has also been considered ([1], [3], [6], [7], [8]). In this work, λ is kept fixed, and the limit $\gamma \to 0$ is carried out under the assumption

$$0 \le U < 2$$

on the contact voltage. An analogous analysis can be carried out for $-2 < U < 0$ but is omitted here for lack of space.

In the following it will be convenient to use the so called quasi Fermi potentials ϕ_n, ϕ_p which are related to the potential and the densities by

$$n = \exp\left(\frac{V - \phi_n - 1}{\gamma}\right), \quad p = \exp\left(\frac{\phi_p - V - 1}{\gamma}\right).$$

These new variables satisfy the formally self-adjoint differential equations

$$\operatorname{div}(n \nabla \phi_n) = 0, \quad \operatorname{div}(p \nabla \phi_p) = 0$$

and the boundary conditions

$$\phi_n = \phi_p = U, \quad \text{on } C_n, \qquad \phi_n = \phi_p = 0, \quad \text{on } C_p.$$

A proof of the following existence result can be found in [4].

Theorem 1. *The problem (1), (2) has a solution which satisfies*

$$\begin{gathered} 0 \le \phi_n, \phi_p \le U, \\ -1 - c\gamma \le V \le U + 1 + c\gamma \end{gathered}$$

where here and in the following c denotes positive constants independent of γ.

For our purposes the value of the estimates in the theorem is limited because they do not imply uniform estimates for the charge carrier densities. Section 2 contains a collection of stronger estimates which are then used in Section 3 for the convergence analysis.

2. A Priori Estimates

Lemma 1. *The derivatives of the quasi Fermi potentials satisfy*

$$\|\nabla\phi_n\|_{L^2(\{V>\phi_n+U-1+2\varepsilon\})} \le c\exp\left(-\frac{\varepsilon}{2\gamma}\right),$$
$$\|\nabla\phi_p\|_{L^2(\{V<\phi_p+1-U-2\varepsilon\})} \le c\exp\left(-\frac{\varepsilon}{2\gamma}\right)$$

for every positive $\varepsilon \le 2-U$.

Outline of a proof. In the nonempty set $\Omega_0 = \{\phi_p - 1 \le V \le \phi_n + U - 1 + \varepsilon\}$, the densities n and p are uniformly bounded. Therefore also ΔV is bounded by the Poisson equation. This can be used to show that Ω_0 is big enough such that there exists a function ϕ_D satisfying the Dirichlet boundary conditions for ϕ_n, such that $\nabla\phi_D$ vanishes in $\{V > \phi_n + U - 1 + \varepsilon\}$ and ϕ_D is uniformly bounded in $H^1(\Omega)$. The estimate for ϕ_n of the lemma then follows from the energy estimate

$$\|\exp\left(\frac{V-\phi_n-U+1-2\varepsilon}{2\gamma}\right)\nabla\phi_n\|_{L^2(\Omega)} \le \|\exp\left(\frac{V-\phi_n-U+1-2\varepsilon}{2\gamma}\right)\nabla\phi_D\|_{L^2(\Omega)}.$$

The second inequality is shown similarly.#

Lemma 2. *The densities n and p are uniformly bounded in $L^\infty(\Omega)$.*

Outline of a proof. Let S denote a component of $\{V > \phi_n + 1\}$. Then the potential satisfies either $V = \phi_n + 1$ or a homogeneous Neumann condition along ∂S. Also,

$$\phi_n = c(\gamma) + O\left(\exp\left(\frac{U-2}{4\gamma}\right)\right), \quad \text{in } S$$

holds with some γ-dependent constant c by the previous lemma (with $\varepsilon = \frac{2-U}{2}$). The maximum principle gives

$$V \le c(\gamma) + 1 + c_1\gamma \le \phi_n + 1 + c_2\gamma$$

implying the boundedness of n in S and therefore in Ω. The boundedness of p is shown analogously.#

A consequence of lemma 2 is the uniform boundedness of ΔV. For the following result we need regularity properties of the boundary. We assume that the boundedness of the densities implies the boundedness of the potential in $H^2(\Omega)$, that extensions of the Dirichlet data as $H^2(\Omega)$-functions exist and that the boundary is a union of segments where the usual trace theorems can be applied.

Lemma 3. *Under the above assumptions we have*

$$\gamma \|\nabla n\|_{L^2(\Omega)} = \|n(\nabla V - \nabla \phi_n)\|_{L^2(\Omega)} \le c\sqrt{\gamma},$$
$$\gamma \|\nabla p\|_{L^2(\Omega)} = \|p(\nabla \phi_p - \nabla V)\|_{L^2(\Omega)} \le c\sqrt{\gamma}.$$

Proof. Let an $H^2(\Omega)$-extension of the Dirichlet data for n be denoted by n_D. Multiplication of the electron continuity equation by $n - n_D$ and integration by parts gives

$$\begin{aligned}\gamma \int_\Omega |\nabla n|^2 d\mathbf{x} &= \gamma \int_\Omega \nabla n . \nabla n_D \, d\mathbf{x} + \int_\Omega n \nabla V . (\nabla n - \nabla n_D) d\mathbf{x} \\ &= -\gamma \int_\Omega n \Delta n_D \, d\mathbf{x} + \gamma \int_{\partial\Omega} n \frac{\partial n_D}{\partial \nu} ds - \int_\Omega \frac{n^2}{2} \Delta V \, d\mathbf{x} \\ &\quad + \int_{\partial\Omega} \frac{n^2}{2} \frac{\partial V}{\partial \nu} ds - \int_\Omega n \nabla V . \nabla n_D \, d\mathbf{x} \le c\end{aligned}$$

where ν denotes the outward unit normal along $\partial\Omega$. The first estimate in the lemma follows immediately, and the second one can be shown similarly.#

3. The limiting problem

The results of the previous section imply that for $\gamma \to 0$ every sequence of solutions has a subsequence such that V converges to V_0 in $C^1(\overline{\Omega}')$ with $\Omega' \subset\subset \Omega$, and n, p, ϕ_n and ϕ_p converge to n_0, p_0, ϕ_{n0} and ϕ_{p0}, respectively, in $L^\infty(\Omega)$-weak *. Our estimates permit passing to the limit in the Poisson equation and in the boundary conditions for V. Therefore,

$$\lambda^2 \Delta V_0 = n_0 - p_0 - C,$$
$$V_0 = U + 1, \quad \text{on } C_n, \qquad V_0 = -1, \quad \text{on } C_p, \qquad \frac{\partial V_0}{\partial \nu} = 0, \quad \text{on } \partial\Omega_N$$

holds. Now we multiply the electron continuity equation by a test function $\varphi \in H_0^1(\Omega \cup \partial\Omega_N)$ and integrate by parts:

$$\int_\Omega \nabla\varphi . (\gamma \nabla n - n \nabla V) d\mathbf{x} = 0$$

Lemma 3 implies that the diffusion term tends to zero as $\gamma \to 0$. From an analogous argument for the hole continuity equation we obtain

$$\operatorname{div}(n_0 \nabla V_0) = 0, \quad \operatorname{div}(p_0 \nabla V_0) = 0.$$

By eliminating the charge carrier densities we arrive at the third order differential equation

$$\operatorname{div}\big((\lambda^2 \Delta V_0 + C)\nabla V_0\big) = 0$$

for the potential. This is a generalization of the equation with $C = 0$ appearing in the so called space charge problem [2]. The difference is the presence of a fixed background charge density. So far we have proven the solvability of this equation subject to the limiting boundary conditions for the potential. However, it is not clear under what circumstances the zero space charge boundary condition

$$\Delta V = 0, \quad \text{on } C_n \cup C_p$$

holds in the limit. The situation is similar to that for the space charge problem where some results are known for special cases [2].

Consider a γ-independent open set S in Ω where the electron density n is uniformly bounded away from zero. Lemma 1 implies that $\nabla\phi_n$ tends to zero in S. On the other hand, the difference between ∇V and $\nabla\phi_n$ vanishes in the limit by lemma 3. Therefore, $\nabla V_0 = 0$ holds in S. It is easy to see that $p_0 = 0$ holds in S. From the limiting Poisson equation we, thus, obtain $n_0 = C$ in S. Since, obviously, n_0 is nonnegative such a set S has to be a subset of the n-region Ω_n. In the same way it can be shown that sets where the limiting hole density p_0 is nonnegative lie in the p-region, that ∇V_0 and n_0 vanish there and that $p_0 = -C$ holds. On the other hand, if $n_0 = p_0 = 0$ holds in an open set, then the limiting potential is a solution of $\lambda^2\Delta V_0 + C = 0$. This suggests that the potential actually solves the equation

$$(\lambda^2\Delta V_0 + C)\nabla V_0 = 0$$

where in the regions with $\nabla V_0 = 0$ we have zero space charge ($n_0 - p_0 - C = 0$), and the regions with $\lambda^2\Delta V_0 + C = 0$ are depletion regions ($n_0 = p_0 = 0$). Recalling that we have $V_0 \in C^1(\Omega)$ and $-1 \le V_0 \le U + 1$ it is obvious that a solution of the limiting problem can be obtained by solving a standard obstacle problem. (For a discussion of its asymptotic behaviour as $\lambda \to 0$ see [8].) However, in general this is not the only solution. Finding additional information which completes a well posed problem for the limiting potential remains the subject of further study.

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