Aplikace matematiky

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Aplikace matematiky, Vol. 32 (1987), No. 1, 49--56

Persistent URL: `http://dml.cz/dmlcz/104235`

32 (1987) APLIKACE MATEMATIKY No. 1, 49—56

ON STEADY-STATE CARRIER DISTRIBUTIONS IN SEMICONDUCTOR DEVICES

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(Received September 2, 1985)

Summary. The author proves the existence of solution of Van Roosbroeck's system of partial differential equations from the theory of semiconductors. His results generalize thsoe of Mock, Gajewski and Seidman.

Keywords: Van Roosbroeck's equations, steady-state carrier distribution semiconductor devices.

INTRODUCTION

In 1950 Van Roosbroeck [12] proposed a system of partial differential equations as a model for the transport of mobile charge carriers in semiconductor devices. The existence of steady-state solutions to Van Roosbroeck's equations (supplemented by reasonable boundary conditions) has been proved under different assumptions by Mock [8, 9] and by Gajewski [4]. A similar result has been obtained by Seidman [10] who dealt with steady-state solutions to diffusion-reaction systems with electrostatic convection. In this paper we shall prove an existence result which generalizes the results of Mock and Gajewski as follows:

1. Van Roosbroeck's equations include (implicitly) a relation between carrier densities and chemical potentials based on Boltzmann statistics. Instead of this we shall use a more general relation special cases of which are the standard relation and a relation based on Fermi-Dirac statistics (cf. Remark 1 below).

2. Carrier mobilities are allowed to depend not only on the electrical field but also on the gradient of the corresponding electrochemical potential. A dependence of this type seems to be quite natural (see, e.g., Selberherr [11], Sect. 4.1).

3. We shall treat boundary conditions allowing the surface charges at insulating gates to depend on the local value of the electrostatic potential.

4. We shall show that one can completely avoid an unpleasant assumption made in the papers quoted above. This assumption reads as follows:

$$(*) \qquad \forall p \geqq 1: \; Bv \in L^p(G) \Rightarrow v \in W^{2,p}(G)\,,$$

where G is the domain occupied by the semiconductor device and B is the second order differential operator with mixed boundary conditions defined below (cf. Section 2). From results of Grisvard [7] it follows that the assumption (*) can be considered as a restriction imposed on the shape of G in connection with the type of the boundary conditions.

Our method of proof is similar to that of the authors mentioned above: A-priori estimates are obtained by means of maximum principle arguments, and the existence of a solution is proved via Schauder's Fixed Point Theorem. In general, steady-state carrier distributions in semiconductor devices are not unique. If, however, the boundary conditions are compatible with vanishing flows then there is a unique solution, the so called thermodynamic equilibrium. This has also been shown by Mock [9] and by Gajewski [4]. In the last section of this paper we shall prove an analogous result under our somewhat more general assumptions. For the sake of simplicity we shall restrict all our considerations to spatially homogeneous semiconductor devices.

1. PROVISIONAL FORMULATION OF THE PROBLEM

Let G be the domain occupied by the semiconductor device. We are looking for functions $u = (u_1, u_2)$, $v = (v_0, v_1, v_2)$ defined on G and sytisfying the following system of equations:

$$(1) \qquad \begin{cases} -\operatorname{div}\left(D_i(|\operatorname{grad} v_0|, |\operatorname{grad} v_i|)\, u_i \operatorname{grad} v_i\right) \\ = k(u)\left(1 - \exp\left(v_1 + v_2\right)\right), \quad u_i = e_i(v_i - q_i v_0), \quad i = 1, 2, \\ -\operatorname{div}\left(\varepsilon \operatorname{grad} v_0\right) = f + u_1 - u_2 ; \end{cases}$$

here

u_1, u_2 represent the densities of holes and electrons,
v_0 represents the electrostatic potential,
v_1, v_2 represent the electrochemical potentials of holes and electrons,
$D_i(|\operatorname{grad} v_0|, |\operatorname{grad} v_i|)$, $i = 1, 2$, are the mobilities of holes and electrons,
ε is the dielectric permittivity of the semiconductor material
f is the net density of charges of ionized impurities,
$k(u)$ is the rate of generation of holes and electrons,
$q_1 = 1$, $q_2 = -1$ represent the charges of holes and electrons,
e_1, e_2 are functions describing the dependence of the carrier densities u_1, u_2 on the corresponding chemical potentials.

Remark 1. If Boltzmann's statistics can be used to model the behaviour of the semiconductor device then

$$e_i(r) = u_0 \exp(r), \quad i = 1, 2,$$

where u_0 is the intrinsic carrier density. If the Fermi-Dirac statistics is necessary to describe the semiconductor then

$$e_i(r) = N_i \mathscr{F}_{1/2}(r - c_i)\,, \quad i = 1, 2\,,$$

where N_i and c_i are given constants (depending on the bandgap and on the densities of states in the conduction band and the valence band), and $\mathscr{F}_{1/2}$ is one of the so called Fermi integrals:

$$\mathscr{F}_{1/2}(r) := \frac{2}{\sqrt{\pi}} \int_0^\infty \sqrt{(s)}\,(1 + \exp(s - r))^{-1}\, ds\,.$$

It is easy to see that $\mathscr{F}_{1/2}(r)$ increases as $r^{3/2}$ provided $r \to +\infty$ and behaves like $\exp(r)$ as $r \to -\infty$. The assumptions on e_i used below are stated in such a way that both examples for e_i mentioned here are admissible. For a detailed physical discussion of these examples we refer to Bonč-Bruevich/Kalašnikov [2].

The equations (1) are to be supplemented by boundary conditions. We assume that the boundary ∂G is the union of two disjoint parts $\tilde{\Gamma}$ and Γ and that

$$(2) \qquad v = \tilde{v} \text{ on } \tilde{\Gamma}\,, \quad \frac{\partial v_0}{\partial \nu} + g(\cdot, v_0) = \frac{\partial v_1}{\partial \nu} = \frac{\partial v_2}{\partial \nu} = 0 \text{ on } \Gamma\,.$$

Here ν denotes the outward unit normal at a point of Γ, and $\tilde{v} = (\tilde{v}_0, \tilde{v}_1, \tilde{v}_2)$ and g are functions describing the interaction of the semiconductor device with its environment. The dot indicates that g may depend on the space variables.

Remark 2. The part $\tilde{\Gamma}$ of the boundary represents the so called ohmic and Schottky contacts whereas Γ represents the insulating parts of the boundary, the insulating gates, and (possibly) the symmetry planes. The function g allows to take into account the surface densities of charges depending on the electrostatic potential. Concrete examples of such functions can be found in Blue-Wilson [1].

2. PRECISE FORMULATION OF THE PROBLEM

With respect to the data of the problem we assume that

$$\text{(A1)} \quad \begin{cases} G \subset \mathbb{R}^N \text{ is a bounded Lipschitzian domain,} \\ \partial G = \tilde{\Gamma} \cup \Gamma,\ \tilde{\Gamma} \cap \Gamma = \emptyset,\ \tilde{\Gamma} \text{ is of positive surface measure;} \end{cases}$$

$$\text{(A2)} \quad \begin{cases} D_i \in C(\mathbb{R}^2_+),\ 0 \leqq m_0(\bar{s} - s) \leqq D_i(r, \bar{s})\,\bar{s} - D_i(r, s)\,s,\ m_0 > 0, \\ D_i(r, s) \leqq m_1, \text{ for } r \geqq 0,\ \bar{s} \geqq s \geqq 0,\ i = 1, 2; \end{cases}$$

(A3) $k \in C(\mathbb{R}^2_+; \mathbb{R}_+)$;

(A4) $f \in L^\infty(G)$, $\varepsilon > 0$ is constant;

(A5) $e_i \in C(\mathbb{R}; \mathbb{R}_+)$ is strictly increasing, $\lim_{r \to \infty} e_i(r) = +\infty$, $i = 1, 2$;

(A6) $\begin{cases} g\colon \Gamma \times \mathbb{R} \to \mathbb{R},\ \forall r \in \mathbb{R}\colon g(\cdot, r) \in L^\infty(\Gamma),\ \forall x \in \Gamma\colon g(x, \cdot) \in C(\mathbb{R}) \text{ is increasing}, \\ g(x, r_0) \geqq 0,\ g(x, -r_0) \leqq 0 \text{ for some } r_0 > 0; \end{cases}$

(A7) $\tilde{v} \in H^1(G; \mathbb{R}^3) \cap L^\infty(G; \mathbb{R}^3)$.

The last assumption means that the function $\tilde{v}$ appearing in (2) can be extended to a function $\tilde{v} \in H^1(G; \mathbb{R}^3) \cap L^\infty(G; \mathbb{R}^3)$.

Let $V := \{w \in H^1(G)\colon w \mid \tilde{\Gamma} = 0\}$, let $\|w\|_V := (\int_G |\text{grad } w|^2 \, dx)^{1/2}$, and let V^* denote the space dual to V. We define operators $A\colon L^\infty(G; \mathbb{R}^2) \times H^1(G; \mathbb{R}^3) \to \to V^* \times V^*$, $F\colon L^\infty(G; \mathbb{R}^3) \to V^* \times V^*$, $B\colon H^1(G) \cap L^\infty(G) \to V^*$ as follows:

$$\langle A(u, v), \hat{h} \rangle := \int_G \sum_{i=1}^{2} D_i(|\text{grad } v_0|, |\text{grad } v_i|)\, u_i \,\text{grad } v_i \,.\, \text{grad } h_i \, dx\,,$$

$$\langle F(u, y), \hat{h} \rangle := \int_G k(u)\,(1 - \exp(y))\,(h_1 + h_2)\, dx\,,$$

$$\langle Bw, h_0 \rangle := \int_G \varepsilon \text{ grad } w \,.\, \text{grad } h_0 \, dx + \int_\Gamma g(\cdot, w)\, h_0 \, d\sigma\,,$$

where $u \in L^\infty(G; \mathbb{R}^2)$, $v \in H^1(G; \mathbb{R}^3)$, $y \in L^\infty(G)$, $w \in H^1(G) \cap L^\infty(G)$, $h_i \in V$, $i = 0, 1, 2$, $\hat{h} = (h_1, h_2)$. By E_i we denote the Nemyckij operator associated with the function e_i, considered as a mapping from $L^\infty(G)$ into itself, $i = 1, 2$.

We are now able to give a precise formulation of the problem stated in Section 1. We are looking for functions $u = (u_1, u_2)$, $v = (v_0, v_1, v_2)$ such that

$$\text{(I)} \quad \begin{cases} u \in L^\infty(G; \mathbb{R}^2)\,, \quad v_i - \tilde{v}_i \in V \cap L^\infty(G)\,, \quad i = 0, 1, 2\,, \\ A(u, v) = F(u, v_1 + v_2)\,, \quad Bv_0 = f + u_1 - u_2\,, \\ u_i = E_i(v_i - q_i v_0)\,, \quad i = 1, 2\,. \end{cases}$$

It is easy to check that for smooth data, sufficiently smooth functions u, v are a solution to Problem (I) if and only if they satisfy (1) and (2). The main result of this paper is

Theorem 1. *If the assumptions* (A1)–(A7) *are satisfied then there exists a solution to Problem* (I).

The proof of this theorem will be given in Section 4.

3. A MODIFIED PROBLEM

Let $K := \max_{i=1,2} \|\tilde{v}_i\|_{L^\infty(G)}$. We fix $M \geqq \max\{\|\tilde{v}_0\|_{L^\infty(G)}, r_0\}$ (cf. (A6)) such that

$$e_1(K - M) - e_2(M - K) + f \leqq 0\,,$$
$$e_1(M - K) - e_2(K - M) + f \geqq 0\,.$$

In view of the assumptions (A4), (A5) this is possible. For $R > 0$ and any real-valued function w we define

$$(P_R w)(x) := \begin{cases} -R & \text{if} \quad w(x) \leqq -R\,, \\ w(x) & \text{if} \quad -R \leqq w(x) \leqq R\,, \\ R & \text{if} \quad w(x) \geqq R\,, \end{cases}$$

for every x from the domain of definition of w. We introduce $B_M: H^1(G) \to V^*$ setting

$$\langle B_M w, h_0 \rangle := \int_G \varepsilon \operatorname{grad} w \,.\, \operatorname{grad} h_0 \, dx + \int_\Gamma g(\cdot, P_M w)\, h_0 \, d\sigma\,,$$

for $w \in H^1(G)$, $h_0 \in V$. In addition to (I) we consider the following "regularized" problem:

$$\text{(II)} \quad \begin{cases} u \in L^\infty(G; \mathbb{R}^2)\,, \quad v - \tilde{v} \in V \times V \times V\,, \\ A(u, v) = F(u, P_K v_1 + P_K v_2)\,, \quad B_M v_0 = f + u_1 - u_2\,, \\ u_i = E_i(P_K v_i - q_i P_M v_0)\,, \quad i = 1, 2\,. \end{cases}$$

Lemma 1. *Let u, v be a solution to Problem* (II). *Then u, v is a solution to Problem* (I) *as well.*

Proof. We shall prove the assertion showing that $\|v_i\|_{L^\infty(G)} \leqq K$, $i = 1, 2$, and $\|v_0\|_{L^\infty(G)} \leqq M$. If w is any real-valued function we denote by w^+, w^- its positive and its negative part, respectively.

1. Let $h_i := (v_i - K)^+$, $i = 1, 2$. Then $h_i \in V$ and $\operatorname{grad} v_i \,.\, \operatorname{grad} h_i = |\operatorname{grad} h_i|^2$ (see, e.g., Gilbarg-Trudinger [6], Sect. 7.4). Therefore $A(u, v) = F(u, P_K v_1 + P_K v_2)$ yields

$$\sum_{i=1}^{2} \int_G \{D_i(|\operatorname{grad} v_0|, |\operatorname{grad} v_i|)\, u_i |\operatorname{grad} h_i|^2 - k(u)\,(1 - \exp(P_K v_1 + P_K v_2))\, h_i\} \, dx = 0\,.$$

The choice of h_i implies that $(1 - \exp(P_K v_1 + P_K v_2))\, h_i \leqq 0$. Moreover (cf. (A2), (A5)),

$$D_i(|\operatorname{grad} v_0|, |\operatorname{grad} v_i|)\, u_i \geqq m_0 e_i(-K - M) > 0\,.$$

Hence

$$\sum_{i=1}^{2} m_0 e_i(-K - M)\, \|h_i\|_V^2 \leqq 0\,.$$

Consequently, $h_i = 0$, i.e., $v_i \leqq K$, $i = 1, 2$. By means of the test functions $(v_i + K)^-$, $i = 1, 2$, one obtains analogously that $v_i \geqq -K$, $i = 1, 2$.

2. Let now $h_0 := (v_0 - M)^+$. Then $h_0 \in V$ and $\operatorname{grad} v_0 \,.\, \operatorname{grad} h_0 = |\operatorname{grad} h_0|^2$. Therefore $B_M v_0 = f + u_1 - u_2$ implies that

$$\int_G \{\varepsilon |\operatorname{grad} h_0|^2 - (f + E_1(v_1 - P_M v_0) - E_2(v_2 + P_M v_0))\, h_0\} \, dx + \\ + \int_\Gamma g(\cdot, P_M v_0)\, h_0 \, d\sigma = 0\,.$$

Because of the choice of h_0 and M we have $g(\cdot, P_M v_0)\, h_0 \geqq 0$ and

$$(f + E_1(v_1 - P_M v_0) - E_2(v_2 + P_M v_0))\, h_0 \leqq$$
$$\leqq (f + e_1(K - M) - e_2(-K + M))\, h_0 \leqq 0\,.$$

Hence

$$\varepsilon \|h_0\|_V^2 = \int_G \varepsilon |\text{grad } h_0|^2 \,\mathrm{d}x \leqq 0\,.$$

This shows that $h_0 = 0$, i.e., $v_0 \leqq M$. Using the test function $(v_0 + M)^-$ one obtains analogously that $v_0 \geqq -M$. This completes the proof.

4. PROOF OF THEOREM 1

We start this section by transforming Problem (II) into a fixed point problem. Subsequently we solve this fixed point problem by means of Schauder's Fixed Point Theorem. Let $H := L^2(G; \mathbb{R}^3)$, and let $\bar{v} \in H$ be given. We define $u = (u_1, u_2) \in L^\infty(G; \mathbb{R}^2)$ by $u_i := E_i(P_K \bar{v}_i - q_i P_M \bar{v}_0)$, $i = 1, 2$. Then we determine v_0 as the solution to

$$B_M v_0 = f + u_1 - u_2\,, \quad v_0 \in V + \tilde{v}_0\,.$$

This is possible since B_M is easily seen to be strongly monotone and continuous on $V + \tilde{v}_0$. After that we determine $\hat{v} = (v_1, v_2)$ as the solution to

$$A(u, v_0, \hat{v}) = F(u, P_K \bar{v}_1 + P_K \bar{v}_2)\,, \quad v_i \in V + \tilde{v}_i\,, \quad i = 1, 2\,.$$

This is possible since $\hat{v} \mapsto A(u, v_0, \hat{v})$ is strongly monotone and continuous on $(V + \tilde{v}_1) \times (V + \tilde{v}_2)$ (cf. [5], Ch. III). We define now $Q: H \to H$ setting

$$Q\bar{v} := v = (v_0, v_1, v_2)\,.$$

Obviously, u, v is a solution to Problem (II) if v is a fixed point of Q and $u_i = E_i(P_K v_i - q_i P_M v_0)$, $i = 1, 2$.

Lemma 2. *The mapping $Q: H \to H$ is continuous. Its range is contained in a convex compact subset of H.*

Proof. 1. The continuity of $Q: H \to H$ can easily be proved by means of the well known continuity properties of Nemyckij operators.

2. With the notation introduced before we have

$$\varepsilon \|v_0 - \tilde{v}_0\|_V^2 \leqq \langle B_M v_0 - B_M \tilde{v}_0, v_0 - \tilde{v}_0 \rangle =$$
$$= \langle f + u_1 - u_2 - B_M \tilde{v}_0, v_0 - \tilde{v}_0 \rangle \leqq$$
$$\leqq c(\|f\|_{L^\infty(G)} + e_1(K + M) + e_2(K + M) + \|B_M \tilde{v}_0\|_{V^*})\, \|v_0 - \tilde{v}_0\|_V\,.$$

Similarly,

$$\sum_{i=1}^{2} m_0 e_i(-K - M) \|v_i - \tilde{v}_i\|_V^2 \leqq \langle A(u, v) - A(u, v_0, \tilde{v}_1, \tilde{v}_2), (v_1, v_2) - (\tilde{v}_1, \tilde{v}_2)\rangle =$$

$$= \langle F(u, P_K\bar{v}_1 + P_K\bar{v}_2) - A(u, v_0, \tilde{v}_1, \tilde{v}_2), (v_1, v_2) - (\tilde{v}_1, \tilde{v}_2)\rangle \leqq$$

$$\leqq c \sup_{\substack{0 \leqq r_i \leqq e_i(K+M) \\ i=1,2}} k(r_1, r_2) (1 + \exp(2K)) \sum_{i=1}^{2} \|v_i - \tilde{v}_i\|_V +$$

$$+ \sum_{i=1}^{2} m_1 e_i(K + M) \|\tilde{v}_i\|_{H^1(G)} \|v_i - \tilde{v}_i\|_V .$$

These results show that $\|v\|_{H^1(G\mathbb{R}^3)}$ is bounded independently of $\bar{v}$. Thus Q maps all of H into a closed ball in $H^1(G; \mathbb{R}^3)$, i.e., into a convex compact subset of H.

Proof of Theorem 1. Lemma 2 shows that there exists a nonempty convex compact subset C of H which is mapped by Q continuously into itself. Thus, Q has a fixed point v by Schauder's Fixed Point Theorem. As mentioned above this implies the existence of a solution to Problem (II). Lemma 1 completes the proof.

5. THERMODYNAMIC EQUILIBRIUM

In general, one cannot expect the solution to Problem (I) to be unique. Special cases in which there exists more than one solution are discussed by Bonč-Bruevich et al. [3]. There is, however, the following simple uniqueness result:

Theorem 2. *Let the assumptions* (A1)–(A7) *be satisfied, and let*

(A8) $$\text{grad}\, \tilde{v}_1 = \text{grad}\, \tilde{v}_2 = 0\,, \quad \tilde{v}_1 + \tilde{v}_2 = 0\,.$$

Then Problem (I) *has a unique solution* u, v. *This solution has the property that* $v_i = \tilde{v}_i$, $i = 1, 2$.

Remark 3. The additional assumption (A8) means that the driving forces for flows vanish at the boundary. The theorem shows that then the flows vanish throughout the device for the unique steady-state solution.

Proof of Theorem 2. Let u, v be a solution to (I). Then

$$0 = \langle A(u, v) - F(u, v_1 + v_2), (v_1, v_2) - (\tilde{v}_1, \tilde{v}_2)\rangle =$$

$$= \int_G \{\sum_{i=1}^{2} D_i(|\text{grad}\, v_0|, |\text{grad}\, v_i|)\, u_i |\text{grad}\, v_i|^2 -$$

$$- k(u) (1 - \exp(v_1 + v_2)) (v_1 + v_2)\}\, dx\,.$$

Since both parts of the integrand are nonnegative this implies that $\text{grad}\, v_i = 0$ and therefore $v_i = \tilde{v}_i$, $i = 1, 2$. Furthermore,

$$Bv_0 = f + E_1(\tilde{v}_1 - v_0) - E_2(\tilde{v}_2 + v_0)\,, \quad v_0 \in V + \tilde{v}_0\,.$$

Because $v_0 \mapsto Bv_0 - E_1(\tilde{v}_1 - v_0) + E_2(\tilde{v}_2 + v)$ is strongly monotone on $V + \tilde{v}_0$ the function v_0 is uniquely determined by the last equation. Finally, the relations $u_i = E_i(v_i - q_i v_0)$, $i = 1, 2$, show that $u = (u_1, u_2)$ is uniquely determined as well.

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Souhrn

O USTÁLENÉM ROZDĚLENÍ NOSIČŮ V POLOVODIČOVÝCH PŘÍSTROJÍCH

Konrád Gröger

Autor dokazuje existenci řešení Van Roosbroeckova systému parciálních diferenciálních rovnic z teorie polovodičů. Jeho výsledky zobecňují výsledky, kterých dosáhl Mock, Gajewski a Seidman.

Резюме

ОБ УСТАНОВИВШЕМСЯ РАСПРЕДЕЛЕНИИ НОСИТЕЛЕЙ В ПОЛУПРОВОДНИКОВЫХ ПРИБОРАХ

Konrád Gröger

Автор доказывает существование решения системы уравнений фан Росбрука в частных производных из теории полупроводников. Его результаты обобщают результаты Мока, Гаевского и Сейдмена.

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