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ON A SHOCKLEY-READ-HALL MODEL FOR SEMICONDUCTORS

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Abstract: *The Shockley-Read-Hall model was introduced in 1952 to describe the statistics of recombination of holes and electrons in semiconductors occurring through the mechanism of trapping and we consider initial-boundary value problems with initial conditions.*

Key words: *partial differential equations, initial-boundary value problems*
AMS subject classification: Primary 35A05. Secondary 35B30

INTRODUCTION

The governing equations are given by

$$\partial_t n = \nabla\left(\mu_n\left(U_T\nabla n - n\nabla V\right)\right) + c_c n_{tr} - c_d n\left(N_{tr} - n_{tr}\right) \tag{1}$$

$$\partial_t p = \nabla\left(\mu_p\left(U_T\nabla p - p\nabla V\right)\right) + c_a n\left(N_{tr} - n_{tr}\right) - c_b n_{tr} p \tag{2}$$

$$\partial_t n_{tr} = c_a\left(N_{tr} - n_{tr}\right) + c_b n_{tr} p - c_c n_{tr} + c_d n\left(N_{tr} - n_{tr}\right) \tag{3}$$

$$\varepsilon_s \Delta V = q\left(n + n_{tr} - p - C\right) \tag{4}$$

Here *n* denotes the density of electrons in the conduction band, whereas *p* is the density of holes in the valence band, with *p*, *n* being opposite charges. The position density of occupied traps is given by n_{tr}; and by c_a, c_b, c_c, c_d we denote the rate constants. The quantity U_T is the so-called thermal voltage. In the following, we consider a semiconductor crystal with a constant (in space) number density of traps N_{tr}.

In the Poisson equation (4), $V(x;\ t)$ is the electrostatic potential, ε_s the permittivity of the semiconductor, *q* the elementary charge, and $C = C(x)$ the doping profile. By adding equations (1),(2),(3), we obtain the continuity equation

$$\partial_t\left(p - n - n_{tr}\right) + \nabla\left(J_n + J_p\right) = 0 \tag{5}$$

with current densities

$$J_n = \mu_n(U_T \nabla n - n\nabla V) \tag{6}$$

and

$$J_p = \mu_p(U_T \nabla p - p\nabla V) \tag{7}$$

Note that for the current density we use the simplest possible model, the drift diffusion ansatz, with constant mobilities μ_n, μ_p. Moreover, as there is no flux, there is no current density J_{tr} .The gap between the valence and the conduction band (which is called the bandgap) is very large for semiconductors, which means that lots of energy is needed to transfer electrons from the valence to the conduction band. This process is referred to as the generation of electron-hole pairs (or pair-generation process), i.e., an electron is created in the conduction band and a hole in the valence band. The inverse process is termed recombination of electron-hole pairs.

We now introduce a rescaling of *n*,*p*, and n_{tr} in order to render the equations (1)-(3) dimensionless: $n \to \overline{C}n$, $p \to \overline{C}p$, $n_{tr} \to N_{tr}$, $C \to \overline{C}C$, $x \to Lx$, $n \to \overline{C}n$, $\mu_{n,p} \to \overline{\mu}\mu_{n,p}$, $n \to \overline{C}n$, $J_{n,p} \to \frac{\overline{\mu}U_T\overline{C}}{L}J_{n,p}$, and $\overline{C}$ is a typical value for *C*. Moreover, we rescale time $t \to \frac{t}{N_{tr}C}$ to make sure that all constants are of order 1, and set $c_c = c_d\overline{C}\,n_0$, $c_d = c_d\frac{\overline{C}}{\tau_n}$, $c_a = c_b\overline{C}\,p_0$, and $c_b = \frac{\overline{C}}{\tau_p}$ .Given the scaling assumption $\varepsilon = \frac{N_{tr}}{C}$ «1, we finally obtain

$$\partial_t n = \nabla J_n + R_n \tag{8}$$

$$\partial_t p = -\nabla J_p + R_p \tag{9}$$

$$\varepsilon\partial_t n_{tr} = R_p - R_n \tag{10}$$

$$\nabla V = n + \varepsilon n_{tr} - p - C \tag{11}$$

where

$$J_n = \mu_n(\nabla n - n\nabla V) \tag{12}$$

and

$$J_p = -\mu_p(\nabla p - p\nabla V)\ . \tag{13}$$

By R_n and R_p we denote the recombination-generation rates for *n* and *p*, respectively:

$$R_n = \frac{1}{\tau_n}(n_0 n_{tr} - n(1 - n_{tr})) \tag{14}$$

$$R_p = \frac{1}{\tau_p}\left(p_0\left(1 - n_{tr}\right) - pn_{tr}\right) \tag{15}$$

Note that $0 \le n_{tr} \le 1$ should hold from physical point of view. Moreover, both *n* and *p* are nonnegative.

MAIN RESULT

We consider initial-boundary value problems with initial conditions

$$n(x,0) = n_I(x), p(x,0) = p_I(x), n_{tr}(x,0) = n_{tr,I}(x) \tag{16}$$

and with mixed Dirichlet-Neumann boundary conditions on $\partial\Omega$, i.e., let

$$n(x,t) = n_D(x), p(x,t) = p_D(x), V(x,t) = V_D(x), x \in \partial\Omega_D \subset \partial\Omega \tag{17}$$

and

$$\frac{\partial n}{\partial \nu} = \frac{\partial p}{\partial \nu} = \frac{\partial V}{\partial \nu} = 0, \partial\Omega_N := \partial\Omega \setminus \partial\Omega_D \tag{18}$$

where ν is the outward unit normal vector along $\partial\Omega_N$ .It is allowed to impose only homogenous Neumann boundary conditions on all of $\partial\Omega$, i.e. we set $\partial\Omega_N = \emptyset$, and the following Theorem will hold.

Theorem Let $n_I, p_I \in L^\infty(\Omega)$ (and non-negative), $0 \le n_{tr,I} \le 1$ and let $C \in L^\infty(\Omega)$. Then, the solution of (8)-(11) satisfies $n, p \in L^\infty_{loc}\left((0,\infty), L^\infty(\Omega) \cap H^1(\Omega)\right)$ and $0 \le n_{tr} \le 1$.

Proof: We will use the result from [5], which was obtained for homogenous Neumann boundary conditions. We can show by a straightforward computation

$$\frac{d}{dt}\int\left[\frac{(n-n_D)^q}{q\mu_n} + \frac{(p-p_D)^q}{q\mu_p}\right]dx =$$

$$= \int\left[\frac{(n-n_D)^{q-1}}{\mu_n}\left(\nabla J_n + R_n - \partial_t n_D\right) + \frac{(p-p_D)^{q-1}}{\mu_p}\left(-\nabla J_p + R_p - \partial_t p_D\right)\right]dx$$

$$\le -(q-1)\int\left[(n-n_D)^{q-2}\nabla(n-n_D)\frac{J_n}{\mu_n} - (p-p_D)^{q-2}\nabla(p-p_D)\frac{J_p}{\mu_p}\right]dx$$

$$+ C_1\int\left(n^q + p^q\right)dx + C_1$$

$$= -(q-1)\int(n-n_D)^{q-2}\nabla(n-n_D)\nabla n dx +$$

$$(q-1)\int(p-p_D)^{q-2}\nabla(p-p_D)\nabla p dx$$

$$+ (q-1)\int[(n-n_D)^{q-2} n\nabla(n-n_D) - (p-p_D)^{q-2} p\nabla(p-p_D)]\nabla V dx$$

$$+C_1\int\left(n^q+p^q\right)dx+C_1$$

$$:=I_1+I_2+I_3+I_4 \tag{19}$$

where the term I_3 from (19) can be rewritten as follows:

$$I_3=\int[(n-n_D)^{q-1}\nabla(n-n_D)-(p-p_D)^{q-1}\nabla(p-p_D)]\nabla V dx+$$

$$+\int[[(n-n_D)^{q-2}\nabla(n-n_D)](n_D\nabla V)-[(p-p_D)^{q-2}\nabla(p-p_D)](p_D\nabla V)]dx$$

$$=-\frac{1}{q}\int[(n-n_D)^q-(p-p_D)^q](n-p+\varepsilon n_{tr}-C)dx$$

$$-\frac{1}{q-1}\int(n-n_D)^{q-1}(\nabla n_D\nabla V+n_D(n-p+\varepsilon n_{tr}-C))dx$$

$$+\frac{1}{q-1}\int(p-p_D)^{q-1}(\nabla p_D\nabla V+p_D(n-p+\varepsilon n_{tr}-C))dx\ .$$

We have used partial integration, and (11) to obtain the last expression. By applying Holder inequality with coefficients *q', r; s* and using the fact that $\frac{1}{q'}+\frac{1}{q}=1$, we obtain the following estimate

$$I_3\le\frac{1}{q}\int\left[(n-n_D)^q-(p-p_D)^q\right](n-n_D-(p-p_D))dx$$

$$+C_2+C_2\int\left(n^q+p^q\right)dx+C_2\|n+p\|_{L^q}^{q-1}\|\nabla n_D\|_{L^r}\ \|n+p\|_{L^q}\ .$$

$\Delta V=\rho, \|\nabla V\|_{L^s}\le C\|\rho\|_{L^q}\|\nabla V\|_{L^s}\le\|\nabla V\|_{W^{1,q}}$,where $\rho=n+\varepsilon n_{tr}-p-C$.

For $q\ge 2$ and even , one obtains for I_1

$$I_1=-\int(n-n_D)^{q-2}|\nabla n|^2dx+\int(n-n_D)^{q-2}\nabla n_D\nabla n dx \tag{20}$$

By rewriting the integrand in the second integral from (20) as

$$(n-n_D)^{q-2}\nabla n_D\nabla n=(n-n_D)^{\frac{q-2}{2}}\nabla n\nabla(n-n_D)^{\frac{q-2}{2}}\nabla n_D \tag{21}$$

and applying the Cauchy-Schwarz inequality, we have the following estimate for (20):

$$I_1\le-\int(n-n_D)^{q-2}|\nabla n|^2dx+\sqrt{\int(n-n_D)^{q-2}\,|\nabla n|^2\,dx\int(n-n_D)^{q-2}|\nabla n_D|^2dx}$$

$$\le\int(n-n_D)^{q-2}|\nabla n|^2dx+\|\nabla n_D\|_{L^q}^2\|n-n_D\|_{L^q}^{q-2} \tag{22}$$

For I_2, the same reasoning (with $n.n_D$ replaced by $p.p_D$, respectively) yields an analogous estimate.

Collecting all the estimates, we finally obtain*:*

$$\frac{d}{dt}\int\left[\frac{(n-n_D)^q}{q\mu_n}+\frac{(p-p_D)^q}{q\mu_p}\right]dx=$$

$$\leq -\frac{1}{2}\int (n-n_D)^{q-2}|\nabla n|^2 dx + \|n_D\|_{L^q}^2 \|n-n_D\|_{L^q}^{q-2}$$
$$-\frac{1}{2}\int (p-p_D)^{q-2}|\nabla p|^2 dx + \|p_D\|_{L^q}^2 \|p-p_D\|_{L^q}^{q-2}$$
$$-\frac{1}{q}\int [(n-n_D)^q-(p-p_D)^q]|\nabla n|^2 (n-n_D-(p-p_D))dx$$
$$+C_3+C_3\int (n^q+p^q)dx + C_3\|n+p\|_{L^q}^{q-1}\|\nabla n_D\|_{L^r}\|n+p\|_{L^q} \quad (23)$$

$$\frac{1}{q}\frac{d}{dt}\left[\|n-n_D\|_{L^q}^q + \|p-p_D\|_{L^q}^q\right]dx \leq \|n_D\|_{L^q}^2 \int |n-n_D|^2 dx + \|p_D\|_{L^q}^2 \int |p-p_D|^q dx$$
$$+C_4\|n+p\|_{L^q}^q + C_4\|n\|_{L^q}^q + C_4\|p_D\|_{L^q}^q$$
$$\leq C_4 2^q \left[\|n-n_D\|_{L^q}^q + \|n_D\|_{L^q}^q + \|p-p_D\|_{L^q}^q + \|p_D\|_{L^q}^q\right] \quad (24)$$

Corollary Given the assumptions of Theorem, consider equations (8)-(11) with homogenous Neumann boundary conditions. Then $n, p \in L^{\infty}_{loc}((0,\infty), L^{\infty}(\Omega)\cap H^1(\Omega))$.

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O SHOCKLEY-READ-HALL MODELU ZA POLUPROVODNIKE

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Apstrakt: *Razmatramo SHOCKLEY-READ-HALL model za poluprovodnike,i dokazuje se granični problem s datim početnim uslovima.*

Ključne reči: *parcijalne diferencijalne jednačine, granični problem*
AMS klasifikacija: Primarna 35B030. Sekundarna 35B30. 35A05.

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