Stability of thermal equilibrium for a semiconductor model including traps

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Abstract. A model for the time dependent behaviour of electrons in semiconductor devices is considered. The model incorporates nonequilibrium effects caused by impurity generated trap levels in the forbidden band. Transport of conduction electrons is modelled by the standard drift-diffusion equation. Existence and uniqueness globally in time of initial-boundary value problems is proven as well as stability of the thermal equilibrium state.

1 Introduction

In semiconductor device simulation the standard models for recombination-generation effects via traps in the forbidden band (see, e.g. [2]) use a quasi steady state assumption for the density of the trapped electrons. This simplification does not permit the modelling of some important transient effects. The present study has been motivated by recent efforts to incorporate nonequilibrium models in semiconductor device simulation software [1]. Detailed proofs of the presented results can be found in [4].

We consider a model for the flow of electrons in a semiconductor crystal incorporating the effects of electron capture and emission by traps in the forbidden band. Also transition processes within the forbidden band are considered. The model consists of the equations

$$\begin{aligned} \frac{\partial n}{\partial t} &= \nabla\cdot(\nabla n - n\nabla V) - R(n,f)\,, \\ \frac{\partial f}{\partial t} &= Q(n,f)\,, \\ \lambda^2\Delta V &= n + n_{tr}(f) - C\,. \end{aligned} \tag{1.1}$$

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Here $f(\boldsymbol{x}, E, t)$ with $0 \le f \le 1$ denotes the portion of occupied traps at position $\boldsymbol{x} \in \Omega \subset \mathbb{R}^3$, energy $E \in (0,1)$ and time $t > 0$. The equations are in dimensionless form, and Ω corresponds to the scaled semiconductor crystal. The energy interval $(0,1)$ is a scaled version of the forbidden band. The density of conduction electrons is denoted by $n(\boldsymbol{x}, t)$ and the operator Q is given by

$$Q(n,f) = \sigma_n \left[\frac{n}{n^*} M(1-f) - f\right] + \int_0^1 \sigma [Mf'(1-f) - M'f(1-f')] N' dE' .$$

Here and in the following we use the notation $g' := g(E')$ for functions of the energy. The first term models emission and capture of conduction electrons, while the integral corresponds to transitions within the forbidden band. The given functions $\sigma_n = \sigma_n(E)$ and $\sigma = \sigma(E, E')$ are scattering cross sections,

$$M = M(E) = \exp\left(-\frac{E}{E_T}\right)$$

is a Maxwellian distribution with the scaled thermal energy E_T, and n^* is a prescribed constant density, characteristic of the semiconductor material. By $N(E)$ we denote the density of states for the traps. The form of Q is determined by using mass action laws for the different transition processes and by the requirement that Q vanishes if f is replaced by the Fermi-Dirac distribution

$$F(n, E) = \left(1 + \frac{n^*}{nM(E)}\right)^{-1} .$$

We also have to assume that σ is symmetric: $\sigma(E, E') = \sigma(E', E)$.

The first equation in (1.1) is the continuity equation for the conduction electrons with the drift-diffusion model $\boldsymbol{J} = \nabla n - n\nabla V$ for the current density where $V(\boldsymbol{x}, t)$ is the electric potential. The source term is defined by

$$R(n,f) = \int_0^1 Q(n,f) N \, dE .$$

This implies conservation of the total number of electrons:

$$\frac{\partial}{\partial t}(n + n_{tr}(f)) = \nabla \cdot \boldsymbol{J} , \qquad n_{tr}(f)(\boldsymbol{x}, t) = \int_0^1 f(\boldsymbol{x}, E, t) N(E) \, dE$$

The last equation in (1.1) is the Poisson equation for the potential with the scaled Debye length λ and the doping profile $C(\boldsymbol{x}) > 0$. The assumption of a positive doping profile is necessary for the validity of the unipolar model (1.1) where the contribution of holes in the valence band is neglected.

We consider initial-boundary value problems with initial conditions

$$n(\boldsymbol{x}, 0) = n_I(\boldsymbol{x}), \qquad f(\boldsymbol{x}, E, 0) = f_I(\boldsymbol{x}, E), \tag{1.2}$$

and boundary conditions

$$\begin{aligned} &n = n_D, \quad V = V_D && \text{on } \partial\Omega_D, \\ &\frac{\partial n}{\partial \boldsymbol{\nu}} = \frac{\partial V}{\partial \boldsymbol{\nu}} = 0 && \text{on } \partial\Omega_N. \end{aligned} \tag{1.3}$$

Here, $\partial\Omega_D \subset \partial\Omega$ denotes the union of contact segments, and $\partial\Omega_N = \partial\Omega \backslash \partial\Omega_D$ the union of insulating and artificial boundary segments. The outward unit normal along $\partial\Omega_N$ is denoted by $\boldsymbol{\nu}$.

Of special interest is the thermal equilibrium problem where the steady state version of (1.1) is considered subject to the boundary conditions (1.3) with the special Dirichlet data $V_D = V_{bi}$ and $n_D = n^* \exp(V_{bi})$. The built-in potential V_{bi} is determined from the algebraic equation

$$n^* e^{V_{bi}} + \int_0^1 F(n^* e^{V_{bi}}, E) N(E)\, dE - C = 0\,.$$

The thermal equilibrium solution satisfies $n_e = n^* \exp(V_e)$, $f_e = F(n_e, E)$ and the semilinear Poisson equation

$$\lambda^2 \Delta V_e = n^* e^{V_e} + \int_0^1 F(n^* e^{V_e}, E) N(E)\, dE - C\,.$$

2 Existence and Uniqueness

The proof of existence and uniqueness relies on rewriting the equation for the conduction electrons by expanding the spatial derivatives and using the Poisson equation:

$$\frac{\partial n}{\partial t} = \Delta n - \nabla n \cdot \nabla V - \frac{1}{\lambda^2}(n - n^-(f))(n - n^+(f))\,,$$

with appropriate definitions of the maps n^- and n^+. A linearized version of the operator Q is defined by

$$
\begin{aligned}
L(n,f,g) &= \sigma_n \frac{n}{n^*} M + \int_0^1 \sigma M f' N' dE' \\
&\quad - g \left[\sigma_n \left(\frac{n}{n^*} M + 1 \right) + \int_0^1 \sigma (M f' + M'(1-f')) dE' \right] .
\end{aligned}
$$

Note that $L(n,f,f) = Q(n,f)$ holds. Now a fixed point operator $(n,f) \longrightarrow (u,g)$ is determined by the following steps: First the infinite system of linear ODE problems

$$
\frac{\partial g}{\partial t} = L(n,f,g)\,, \qquad g(\boldsymbol{x},E,0) = f_I(\boldsymbol{x},E) \tag{2.1}
$$

is solved. Then the electrostatic potential is determined from

$$
\lambda^2 \Delta V = n + n_{tr}(g) - C\,, \qquad V = V_D \text{ on } \partial\Omega_D\,, \quad \frac{\partial V}{\partial \boldsymbol{\nu}} = 0 \text{ on } \partial\Omega_N\,. \tag{2.2}
$$

Finally the update for the electron density solves the linear initial boundary value problem

$$
\begin{aligned}
\frac{\partial u}{\partial t} &= \Delta u - \nabla u \cdot \nabla V - \frac{1}{\lambda^2}(u - n^+(g))(n - n^-(g))\,, \qquad (2.3) \\
u &= n_D \text{ on } \partial\Omega_D\,, \qquad \frac{\partial u}{\partial \nu} = 0 \text{ on } \partial\Omega_N\,, \\
u(\boldsymbol{x},0) &= n_I(\boldsymbol{x})\,.
\end{aligned}
$$

Maximum principles for (2.1) and (2.3) imply that the fixed point operator maps a set, bounded with respect to the L^∞-norm uniformly in time, into itself. Also, for short times, the fixed point map is a contraction. These are the main ingredients of the proof of

Theorem 2.1 *Under appropriate smoothness and boundedness assumptions on the data (see [4]) the problem (1.1), (1.2), (1.3) has a unique solution for all $t > 0$. Also there exist constants $0 < \underline{n} \le \overline{n}$ such that*

$$
\underline{n} \le n(\boldsymbol{x},t) \le \overline{n}\,, \qquad F(\underline{n},E) \le f(\boldsymbol{x},E,t) \le F(\overline{n},E)\,.
$$

3 Stability of thermal equilibrium

We first examine the linearized stability of the equilibrium solution. Extending ideas of Mock [3] we make the ansatz

$$\begin{aligned} V &= V_e + \omega(\boldsymbol{x}) e^{\mu t}\,, \\ n &= n_e + n_e(\omega(\boldsymbol{x}) - \alpha(\boldsymbol{x})) e^{\mu t}\,, \\ f &= f_e + f_e(1-f_e)(\omega(\boldsymbol{x}) - \beta(\boldsymbol{x},E)) e^{\mu t}\,. \end{aligned} \tag{3.1}$$

Then the linearized version of (1.1) reads

$$\begin{aligned} \mu n_e(\omega - \alpha) &= -\nabla \cdot (n_e \nabla \alpha) + \int_0^1 \sigma_n f_e (\alpha - \beta) N \, dE\,, \\ \mu f_e(1-f_e)(\omega - \beta) &= \sigma_n f_e(\beta - \alpha) + e^{-V_e} \int_0^1 \sigma f_e f_e' (\beta - \beta') N' \, dE'\,, \\ \lambda^2 \Delta \omega &= \omega\Big(n_e + n_{tr}(f_e(1-f_e))\Big) - n_e \alpha - n_{tr}(f_e(1-f_e)\beta)\,. \end{aligned}$$

The particular form of (3.1) has two important consequences: The spatial operator in the first equation is formally self-adjoint, and the potential contribution ω does not appear in the linearized recombination-generation terms. Manipulations similar to those used by Mock [3] lead to the following result (see [4] for further details):

Theorem 3.1 *Under the assumptions of theorem 2.1 all eigenvalues of the linearization of (1.1), (1.3) at the thermal equilibrium solution are real and negative.*

For a nonlinear stability result we need two additional technical assumptions: Let the doping profile C be constant and

$$n^* \geq \int_0^1 MN \, dE\,.$$

Theorem 3.2 *Let the above assumptions be satisfied and let the initial data n_I and f_I be uniformly close enough to the equilibrium solution n_e and f_e. Then the solution of (1.1), (1.2), (1.3) with thermal equilibrium boundary conditions converges to the equilibrium solution as $t \to \infty$.*

For the proof the ideas of the linearized stability analysis are used. The nonlinear terms can be controlled by tedious but rather straightforward estimates.

4 Conclusions

A semiconductor model including the nonequilibrium behaviour of trapped electrons has been found to be mathematically well posed. Also the stability of the thermal equilibrium solution has been proven, a necessary condition for the plausibility of the model. The present analysis could serve as a starting point for a mathematically rigorous understanding of some of the interesting dynamical behaviour of semiconductors induced by recombination-generation effects [5]. In this context, this work should be extended in two directions. First, bipolar models (including the transport of holes) should be considered. Second, the stability of nonequilibrium steady state solutions should be investigated.

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