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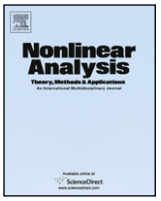

Classical solutions of drift–diffusion equations for semiconductor devices: The two-dimensional case

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ABSTRACT

We regard drift–diffusion equations for semiconductor devices in Lebesgue spaces. To that end we reformulate the (generalized) van Roosbroeck system as an evolution equation for the potentials to the driving forces of the currents of electrons and holes. This evolution equation falls into a class of quasi-linear parabolic systems which allow unique, local in time solution in certain Lebesgue spaces. In particular, it turns out that the divergence of the electron and hole currents is an integrable function. Hence, Gauss' theorem applies, and gives the foundation for space discretization of the equations by means of finite volume schemes. Moreover, the strong differentiability of the electron and hole density in time is constitutive for the implicit time discretization scheme. Finite volume discretization of space, and implicit time discretization are accepted custom in engineering and scientific computing. This investigation puts special emphasis on non-smooth spatial domains, mixed boundary conditions, and heterogeneous material compositions, as required in electronic device simulation.

1. Introduction

In 1950 van Roosbroeck [1] established a system of partial differential equations describing the motion of electrons and holes in a semiconductor device due to drift and diffusion within a self-consistent electrical field, see also [2–7]. In 1964 Gummel [8] published the first report on the numerical solution of these drift–diffusion equations for an operating semiconductor device. From that time on, van Roosbroeck's system has been the backbone of many a model in semiconductor device simulation. The first papers devoted to the mathematical analysis of van Roosbroeck's system appeared in the early seventies of the previous century [9,10]; for a historical synopsis and further references see [5]. Recently Markowich et al. [11] have shown global existence and asymptotic behavior of solutions in the whole space case. In 1986 Gajewski and Gröger proved the global existence and uniqueness of weak solutions under realistic physical and geometrical conditions [12]. The key for proving these results and also for establishing stable numerical solving procedures is the existence of a Lyapunov function for the van Roosbroeck system. This solution theory entails restricting conditions on the models for the recombination of electron–hole pairs, see [5 (2.2.3),13 (Ch. 5),14 (Ch. 6),15,16]. In this paper we relax the condition on the reaction terms in the equations considerably, up to the point that some external control to the generation or annihilation of electrons or holes can be applied individually. In particular, this aims at radiative recombination of electron–hole pairs in semiconductor lasers, and at the generation of electron–hole pairs in optoelectronic detectors. Notwithstanding this generalization, we continue to use the name van Roosbroeck system for the model equations.

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Van Roosbroeck's system consists of current-continuity equations — one for electrons, another one for holes — which are coupled to a Poisson equation for the electrostatic potential, and comprise generative terms, first of all recombination of electron–hole pairs. The current-continuity equations can be viewed as quasi-linear parabolic equations. However, the natural formulation of balance laws is in integral form

$$\frac{\partial}{\partial t}\int_\omega u_k \,\mathrm{d}x = \int_{\partial\omega} \nu \cdot j_k \,\mathrm{d}\sigma_\omega + \int_\omega r_k \,\mathrm{d}x. \tag{1}$$

Here u_2 and u_1 is the density of electrons and holes, respectively, j_k is the corresponding flux, and r_k is a reaction term. ω is any (suitable) sub-domain of the whole domain under consideration, ν is the outer unit normal to the boundary $\partial\omega$ of ω and σ_ω is the arc measure on $\partial\omega$. In the weak formulation of the balance law the boundary integral of the normal component of the current is expressed as the volume integral of the divergence of the corresponding current. Very little is known about the question whether the weak solutions also satisfy the original balance law equations (1). Obviously, this depends on the applicability of Gauss' theorem. So, the problem is about the divergence of the currents in weak solutions being functions — not only distributions. In particular, this comes to bear in the numerical treatment of van Roosbroeck's system. The choice for space discretization of drift–diffusion equations is the finite volume method, see [17], which rests on the original balance law formulation (1) of the equations.

In this paper we solve this problem for the spatially two-dimensional van Roosbroeck system by showing that it admits a classical solution in a suitably chosen Lebesgue space—at least locally in time. Aiming at the inclusion of rather general recombination and generation processes for electron–hole pairs we cannot expect global existence anymore, and we cannot rely on a Lyapunov function. Instead we apply local methods for quasi-linear evolution equations. To that end, we rewrite van Roosbroeck's system as an evolution equation for the electrochemical potentials of electrons and holes, and apply a recently obtained result on quasi-linear parabolic equations in Lebesgue spaces, see [18]. This yields a classical solution of van Roosbroeck system locally in time with currents the divergence of which is Lebesgue integrable to some exponent greater than one. The strong differentiability of the electron and hole density in time is constitutive for the implicit time discretization scheme which is accepted custom in engineering and scientific computing, see for instance [5].

Please note that in device simulation one is always confronted with contacted devices of heterogeneous material composition. That leads to mixed boundary conditions and jumping material coefficients in the model equations. Hence, standard theorems on existence, uniqueness and regularity do not apply.

2. Van Roosbroeck's system

Basic variables

In the following we investigate van Roosbroeck's model for a semiconductor device which describes the flow of electrons and holes in a self-consistent electrical field due to drift and diffusion. The physical quantities one is interested in are: the densities u_1 and u_2 of holes and electrons, the densities j_1 and j_2 of the hole and electron currents, the electrostatic potential $\widetilde{\varphi}$ of the self-consistent electrical field, and the electrochemical potentials $\widetilde{\phi}_1$ and $\widetilde{\phi}_2$ of holes and electrons. These unknowns have to satisfy Poisson's equation and the current-continuity equations for electrons and holes with some side conditions. The latter are given by the relations between the potentials and the densities.

Spatial domain

We study only semiconductor devices which are quasi-translational invariant in one space direction or angular symmetric. In that case van Roosbroeck's system in real space can be reduced to a similar set of equations in the plane. That means, we regard a cut through the device perpendicular to the direction of invariance. Let $\widehat{\Omega}$ be the resulting two-dimensional (bounded) representative domain. Parts of the device may be insulating, for instance formed by an oxide. Then, electrons and holes can move only in a sub-domain Ω of $\widehat{\Omega}$. This also covers the case of charges which are artificially immobilized on a sub-domain $\widehat{\Omega} \setminus \Omega$. Furthermore, we mark out a part $\widehat{\Gamma}$ of the boundary of $\widehat{\Omega}$ where the device borders on an insulator. The remaining part of the boundary represents (possibly several) contacts of the device. We also mark out a part Γ of Ω's boundary. In the case of a stand-alone drift–diffusion model of the semiconductor device again Γ represents areas of the device bordering to an insulator, whereas the remaining part is the contact area.

External control

In real-world modeling of semiconductor devices van Roosbroeck's system often serves as a component in a compound model of the device. Then the superordinated system – for instance a circuit model – may exercise a control on van Roosbroeck's system. Apart from a superordinated circuit model, compound models comprising in addition to van Roosbroeck's system equations for the lattice temperature or the power of lasing modes play an important role in device simulation, see for instance [5,19–21]. But the concept of external control also comes to bear in segmentation of the simulation domain, in particular in connection with multiscale modeling, see for instance [22–24].

If van Roosbroeck's equations serve as a component of a compound model, then system parameters, state equations, boundary conditions, et alii, possibly bear a different physical meaning than in the stand-alone model.

We make assumptions about an external control from the initial time T_0 up to a time T_1.