

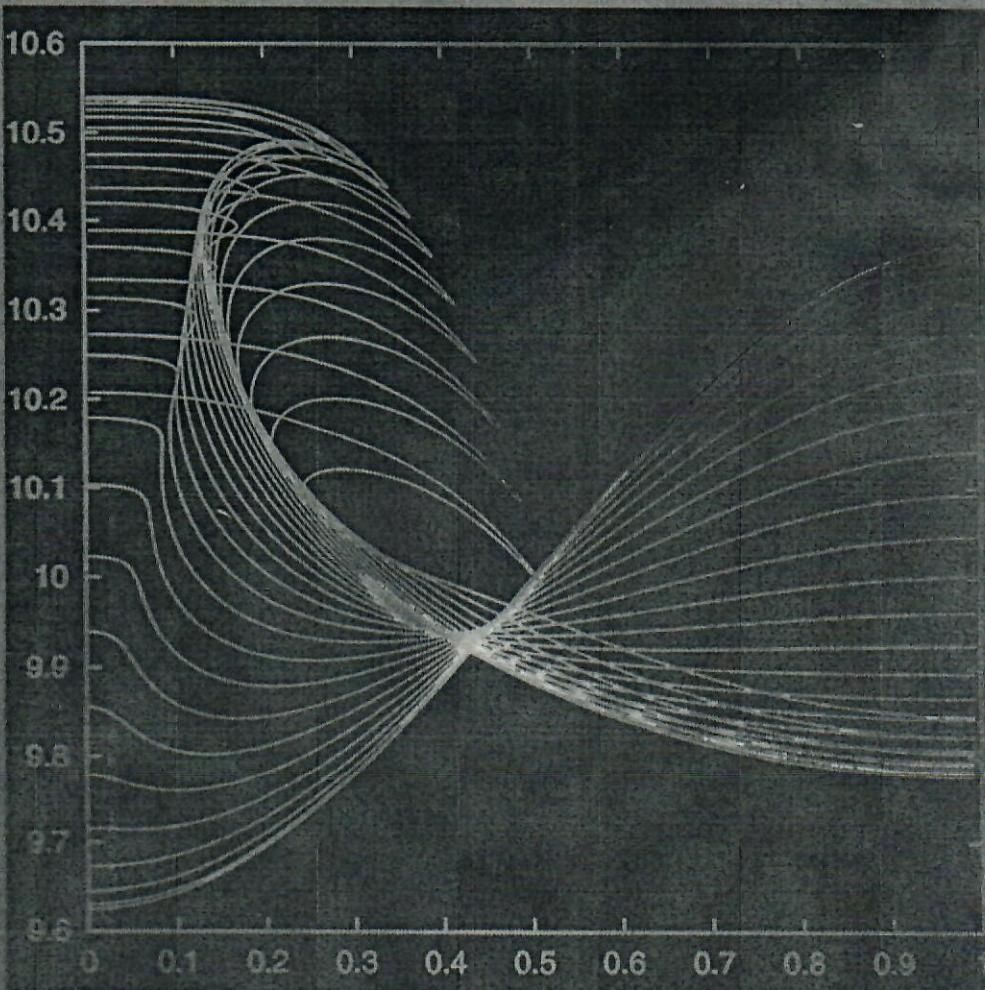
Noye
Teubner
Gill

COMPUTATIONAL TECHNIQUES
AND APPLICATIONS: CTAC97

Proceedings of the Eighth Biennial Conference

**COMPUTATIONAL
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Editors: **John Noye, Michael Teubner & Andrew Gill**



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COMPUTATIONAL TECHNIQUES AND APPLICATIONS: CTAC97

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Editors

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Preface

This volume contains papers presented at the Conference on Computational Techniques and Applications (CTAC97) held in Adelaide, South Australia from 10-14 August 1997.

The CTAC series of conferences on Computational Mathematics and Applications (ANZIAM) began in 1973. It is a forum for scientists and engineers to present their computational techniques and applications.

Previous CTAC conferences were held at the University of Queensland, Brisbane (1973), University of New South Wales, Kensington (1975),

Five invited speakers presented their papers without charge.

Graham Carey (UCL), Michael Powell (UCL), Alan Stroud (Dimensions), Alshai Runchal (Aerojet General), Ernie Tuck (University of New South Wales), Boundary and Detonation, Daniel Yuen (BHP)

In addition to the invited speakers, there were about 150 other participants at the conference. The topics covered comprised about 100 papers. Most of the papers concerned with numerical methods for the solution of partial differential equations were concerned with finite difference and finite element methods. There was also a range of topics concerned with the modelling of physical processes such as combustion, jetted foodstuffs, oil spills, and wave propagation in coastal seas. The implementation of numerical methods for problems involving discontinuous solutions was also considered.

A half day workshop on the numerical solution of inverse problems was held on the Wednesday afternoon. This workshop was well attended by C

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Modelling of Nonlocal Physical Effects in Semiconductor Plasma Using Quasi-Hydrodynamic Models

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1. Introduction

Computational microelectronics is an area of science where application of mathematics may be considered only as a two-way interaction between mathematical and physical-technological models. Problems of plasmo-chemical etching, crystal growth, ion lithography, and of the description of processes of fluid and gas epitaxy, and of electron-hole plasma in semiconductor devices give just a few examples of today's challenging problems in this rapidly growing field where mathematical tools essentially determine the technological progress.

On the one hand, microelectronics provides a wide range of challenging mathematical problems that, in their complexity, are comparable with such long standing scientific problems as climate modelling. On the other hand, since the computational experiment is at the heart of applications of mathematical modelling in microelectronics, we have to have a sufficient element base and hardware (which may be provided by microelectronics) for such an experiment to succeed. This "circle" of interdependencies between computational experiments and physical-technological designs leads one to view the process of mathematical modelling in a broader sense implying the necessity of the consideration of a *hierarchy* of mathematical models, perhaps with overlapping "borders" of applicability. Application of a particular model in such a hierarchy significantly increases the importance of the effectiveness of algorithms used in computational experiments.

In this paper we deal with the one class of problems in computational microelectronics, namely semiconductor device modelling. For this purpose a hierarchy of mathematical models may be constructed within the framework of the relaxation time concept. While neglecting relaxation time may still provide a sufficient approximation in many classical areas of mathematical modelling, it is not so for many important problems in computational microelectronics. Mathematically, the relaxation time, τ , is introduced through a highly non-regular function of the scattering (or transition) rate (denoted by s) as

$$\tau(x, v) = 1 / \int_B s(x, v, v') dv' , \quad (1.1)$$

where v denotes the velocity function, and the integral is taken over the Brillouin zone \mathcal{B} of the lattice. Such a function enters implicitly the Boltzmann-type equation for carrier transport through the collision operator in the right-hand side (see, for example, [2]). The non-zero relaxation time prohibits a theoretically possible situation of infinite velocity propagation and, in the end, allows us to satisfy the Pauli principle.

We organise this paper as follows.

- In Section 2 we consider models from a hierarchy of mathematical models for charge transport in semiconductors. Such a hierarchy depends on the role of collisions between charge carriers compared to other mechanisms of scattering.
- Section 3 is devoted to a nonlocal model of this hierarchy known as the quasi-hydrodynamic model.
- In Section 3 we address the issues of the construction and investigation of exponential difference schemes of semi-implicit type for non-local models of semiconductors.
- Some numerical results are presented in Section 4. Conclusions and future directions are also discussed.

2. Relaxation Time in a Hierarchy of Mathematical Models

In the context of semiconductor device modelling the relaxation time τ may be considered as an average time between subsequent collisions of carriers with each other (the quantity that characterises the velocity of exchange by both quasi-impulse and energy). If we also introduce times that describe exchange of energy and quasi-impulse between carriers and crystal lattice of a semiconductor as τ_ω and τ_p respectively, then it is natural to distinguish the two limiting cases:

- when the scattering of carriers by collision is not essential and the charge carriers cannot be considered as an independent thermodynamical system due to scattering on the lattice imperfections, i.e. when

$$\tau_p \leq \tau_\omega \ll \tau \text{ or } \tau_p \approx \tau_\omega \ll \tau, \quad (2.1)$$

- when carriers have enough time to exchange energy and quasi-impulse before scattering on lattice imperfections plays the essential role (a weak interaction with the lattice allows us to consider the system as an almost independent thermodynamical system), i.e. when

$$\tau \ll \tau_p \ll \tau_\omega \quad (2.2)$$

Limiting situations (2.1), (2.2) restrict our consideration to *kinetic* and *hydrodynamic* models respectively, and do not cover an important case when charge carriers have enough time to exchange energy (but not quasi-impulse!) before the scattering on the lattice imperfections becomes essential. This situation, when

$$\tau_p \leq \tau \ll \tau_\omega \text{ or } \tau_p \approx \tau \ll \tau_\omega, \quad (2.3)$$

leads us to the consideration of quasi-hydrodynamic models (QHM) for semiconductors.

Strictly speaking, the times τ , τ_ω and τ_p may not be overlapping. For example, on the Hilbert expansion model to a model of the kinetic theory scaling for the time between the collision and the scattering of carriers, the model from hydrodynamics is mapped directly to the exact solution of the impulse conservation equation.

The standard theory of hydrodynamic models for carrier densities assumes the dependency between the times τ , τ_ω and τ_p that is often expressed by the model from such a way that the effective temperature and the electro-magnetic field in plasma often rest on the application of the theory.

3. Quasi-Hydrodynamic Models

We consider a one-dimensional model which after appropriate transformation

where the current density is given by

$$J_n = \int_{\mathcal{B}} v_n n \, d\mathbf{v}$$

$$Q_n = \beta_n T_n n \mu$$

The system is closed by the boundary conditions $T_1 = T_2 = T$ and is supplemented by the condition $\int_{\mathcal{B}} \mathbf{v} \cdot \mathbf{n} Q_n \, d\mathbf{v} = 0$.

$$n(x, t) = \int_{\mathcal{B}}$$

and boundary conditions $n(x, 0) = n_0$ and $\partial_n n(x, t) = 0$.

(it is also assumed that $\mu = \mu_0$ and $\beta_1 = \beta_2 = \beta$), the boundary conditions $\varphi(0, 0) = \varphi_0$ and $\partial_n \varphi(0, t) = 0$.

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Strictly speaking, the borders of applicability of these three classes of models may not be overlapping. The standard techniques (such as perturbation arguments based on the Hilbert expansion or the method of moments) for the "reduction" of the kinetic model to a model of the hydrodynamic type require, in the end, the choice of the time scaling for the transport equation that will define an approximate relationship between the collision operator and the driving force. The principal difference of our model from hydrodynamic models is in coupling the equation(s) of carrier motion directly to the energy equation(s) without the requirement for a coupling to the impulse conservation equation(s).

The standard techniques (mentioned above) provide a tool for the reduction of hydrodynamic model to the drift-diffusion model (DDM) under the assumption of low carrier densities and small electro-magnetic fields. The key issue of such a reduction is the dependency between the mobilities of the drift terms with the diffusion coefficients that is often expressed by the Einstein-type relation. The principal difference of our model from such drift-diffusion models is in the fact that the mobility (and so the effective temperature) become a function of carrier energy rather than local value of electro-magnetic field strength. The nonequilibrium behaviour of the semiconductor plasma often restricts, and in many cases completely excludes, the possibility of application of the classical drift-diffusion models.

3. Quasi-Hydrodynamic Models for Semiconductors

We consider a non-local quasi-hydrodynamic model for the two-type carrier case, which after appropriate scaling (see [3] and references therein) has the following form

$$\begin{cases} \partial_{xx}\varphi = n - p - N, \\ \partial_t n - \partial_x J_n = F, \\ 3/2\partial_t(nT_n) + \partial_x Q_n = -J_n\partial_x\varphi + P_n, \\ \partial_t p + \partial_x J_p = F, \\ 3/2\partial_t(pT_p) + \partial_x Q_p = J_p\partial_x\varphi + P_p, \end{cases} \quad (3.1)$$

where the current and energy flux are given by

$$J_n = -n\mu_n\partial_x\varphi + \partial_x(T_n\mu_n n), \quad J_p = -p\mu_p\partial_x\varphi - \partial_x(T_p\mu_p p), \quad (3.2)$$

$$Q_n = \beta_n T_n n \mu_n \partial_x \varphi - \beta_n \partial_x [T_n D_n n], \quad Q_p = -\beta_p T_p p \mu_p \partial_x \varphi - \beta_p \partial_x [T_p D_p p]. \quad (3.3)$$

The system is considered in the space-time region $\bar{G} = \{(x, t) : 0 \leq x \leq 1, 0 \leq t \leq T\}$ and is supplemented by the initial

$$n(x, 0) = n_0(x), \quad p(x, 0) = p_0(x), \quad T_n(x, 0) = T_p(x, 0) = 1, \quad (3.4)$$

and boundary conditions

$$p - n + N = 0, \quad pn = n_{ie}^2, \quad T_n = T_p = 1, \quad \varphi = \varphi_0 \quad (3.5)$$

(it is also assumed that the condition $J_n(x, 0) = J_p(x, 0) = 0$ and the conjugating conditions $\varphi(0, 0) = 0, \varphi(1, 0) = \varphi_0$ are satisfied).

In (3.1)–(3.5), n and p denote the concentration of majority and minority carriers in a two-type carrier semiconductor (and n_0, p_0 are initial concentrations); T_n and T_p denote their temperatures; F denotes the recombination-generation function; N is the dopant distribution in the semiconductor; φ denotes the potential of the electric field (and φ_0 is the sum of the contact potential and the applied voltage); n_{ie} is the effective intrinsic concentration of carriers; β_n and β_p are the Peltier coefficients; μ_n (μ_p) and D_n (D_p) denote the mobility and diffusion coefficient of the majority (minority) carriers.

4. Difference Schemes for Nonlocal Models of Quasihydrodynamic Type

One of the major problems in the construction of effective numerical schemes for semiconductor device modelling is to guarantee the stability of numerical procedures for abruptly changing coefficients. The first step in the achievement of this goal is the construction of *monotone difference schemes*.

In the space-time region \tilde{G} we introduce a non-uniform grid $\hat{\omega}_{h\tau} = \hat{\omega}_h \times \hat{\omega}_\tau$ and we will compute the values of φ, n, p, T_n , and T_p in the “whole” nodes whereas the values of J_n, J_p, Q_n, Q_p , and $E = -\nabla\varphi$ will be computed in the data-driven (“flux”) nodes (i.e. $x_{i+1/2}, i=1,\dots,N-1$). Other notation are standard for theory of difference scheme (see, for example, [5] and references therein).

Mathematical difficulties caused by the problem of approximation of current density are well known since the publication of the first paper by Gummel on this topic. Indeed the application of standard approximations (even in the case of the classical DDM) is impeded by the very restrictive condition on the space step discretization which follows from the *maximum principle* [3]. These difficulties may be overcome when in addition to the monotonicity property we construct difference schemes that are usually referred to as *exponential*. For example, we may approximate the current density of the majority carriers as follows

$$J_{i+1/2} = \frac{1}{h_{i+1}} \left[D(T_{i+1}) n_{i+1} f_1 \left(\frac{\varphi_{i+1} - \varphi_i}{T_{i+1/2}} \right) - D(T_i) n_i f \left(\frac{\varphi_{i+1} - \varphi_i}{T_{i+1/2}} \right) \right], \quad (4.1)$$

where

$$f(x) = xe^x/(e^x - 1), \quad f_1(x) = x/(e^x - 1) \quad (4.2)$$

are Bernoulli functions ($f_1(x) = f(-x)$). As we may expect, approximation (4.1) turns into the classical Scharfetter-Gummel approximation when $T_{i+1} \rightarrow T_i$.

However, the attempts to generalise this idea into the energy equation(s) in the case of QHM lead to serious mathematical difficulties. In fact, the analysis conducted for the stationary problems (see [3] and references therein) showed that the resulting approximations for the energy balance equations imply a quite severe restriction (in particular, for strong electric fields) on space discretisation, namely,

$$h < 2\beta/E^*, \text{ where } E^* = \max_{i=1,2,\dots,N} |E_{i+1/2}|, \quad \beta = \min\{\beta_n, \beta_p\}. \quad (4.3)$$

Such difficulties are cased by the fact that in contrast to the continuity equations, the energy balance equation(s) cannot be cast in the “divergence” form since it (they)

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contain(s) non-selfconjugate operators. Nevertheless, it is possible to transform the expression for the energy flux to the form where all derivatives of energy functions ($\mathcal{E}_n = nT_n$ and $\mathcal{E}_p = pT_p$) enter under the sign of divergence in the flux term. For example, for the balance energy equation for the majority carrier system we have

$$3\partial_t \mathcal{E}_n/2 = \partial_x Q_n^* + S_n(T_n, \varphi) \mathcal{E}_n, \quad (4.4)$$

where

$$\mathcal{E}_n = nT_n, \quad S_n = \mu_n(T_n)\partial_{xx}\varphi + \mu_n(T_n)(\partial_x\varphi)^2/T_n + (1 - T_n)/(\tau_\omega^n(T_n)T_n), \quad (4.5)$$

$$Q_n^* = \beta_n \partial_x(D_n(T_n)\mathcal{E}_n) - (1 + \beta_n)\mu_n(T_n)\mathcal{E}_n \partial_x\varphi \quad (4.6)$$

(here τ_ω^n [τ_ω^p] are characteristic times of energetic relaxation).

Representation (4.4)–(4.6) allows us to construct monotone exponential schemes which are not necessarily conservative. Leaving out the details, in the nonstationary case we get the following scheme constructed on the non-uniform grid $\hat{\omega}_{h\tau}$:

$$(n_i^{l+1} - n_i^l)/\tau_{l+1} = [A_i^n n_{i-1}^{l+1} + B_i^n n_{i+1}^{l+1} - C_i^n n_i^{l+1}] + F_i, \quad (4.7)$$

where

$$A_i^n = \frac{D_n[(T_n)_{i-1}^{l+1}]}{h_i} f\left(\frac{\varphi_i^{l+1} - \varphi_{i-1}^{l+1}}{(T_n)_{i-1/2}^{l+1}}\right), \quad B_i^n = \frac{D_n[(T_n)_{i+1}^{l+1}]}{h_{i+1}} f_1\left(\frac{\varphi_{i+1}^{l+1} - \varphi_i^{l+1}}{(T_n)_{i+1/2}^{l+1}}\right), \quad (4.8)$$

and $C_i = A_{i+1}^n + B_{i-1}^n$ (note that when splitting methods are used, the value of n^{l+1} in F can be found from the approximation of the Poisson equation, $\Delta\varphi = n^{l+1} - p^{l+1} - N$, but in this case the values of p are forced to be taken from the time layer l). Using similar transformations, we also get the exponential difference scheme for the continuity equation for the minority carrier system.

Now we are in the position to consider much more difficult equations for energy balance. First, we reduce these equations to the "quasi-conservative" forms, for example, for an electron system we have

$$3/2\partial_t \mathcal{E}_n = \beta_n \partial_{xx}[D_n(T_n)\mathcal{E}_n] - (1 + \beta_n)\partial_x[\mu_n(T_n)\mathcal{E}_n \partial_x] \\ + \mu_n(T_n)\mathcal{E}_n \partial_{xx}\varphi + \mathcal{E}_n \mu_n(T_n)(\partial_x\varphi)^2/T_n - \mathcal{E}_n(1 - 1/T_n)/(\tau_\omega^n(T_n)) \quad (4.9)$$

As a result of transformations analogous to those performed for the continuity equation we get the following difference scheme

$$\frac{3}{2} \frac{(\mathcal{E}_n)_i^{l+1} - (\mathcal{E}_n)_i^l}{\tau_{l+1}} = (\Lambda_{T_n}(\varphi^{l+1}, T_n^{l+1})\mathcal{E}_n^{l+1})_i, \quad (4.10)$$

where

$$(\Lambda_{T_n}(\varphi, T_n)\mathcal{E}_n)_i = \{\bar{A}_i^n(\mathcal{E}_n)_{i-1} + \bar{B}_i^n(\mathcal{E}_n)_{i+1} - \bar{C}_i^n(\mathcal{E}_n)_i\}/h_i^* - \{-\mu_n[(T_n)_i]\varphi_{xx,i} - \\ \mu_n[(T_n)_i](\varphi_{xx,i})^2/(T_n)_i + +1/\tau_\omega^n[(T_n)_i] - 1/(\tau_\omega^n[(T_n)_i](T_n)_i)\}(\mathcal{E}_n)_i, \quad (4.11)$$

and the coefficients of this difference scheme are defined as follows

$$(\tilde{A})_i^n = \frac{\beta_n D_n [(T_n)_{i-1}^{l+1}]}{h_i} f \left(\frac{1 + \beta_n \varphi_i^{l+1} - \varphi_{i-1}^{l+1}}{\beta_n (T_n)_{i-1/2}^{l+1}} \right), \quad (4.12)$$

$$(\tilde{B})_i^n = \frac{\beta_n D_n [(T_n)_{i+1}^{l+1}]}{h_{i+1}} f_1 \left(\frac{1 + \beta_n \varphi_{i+1}^{l+1} - \varphi_i^{l+1}}{\beta_n (T_n)_{i+1/2}^{l+1}} \right), \quad (4.13)$$

and $\tilde{C}_i^n = \tilde{A}_i^n + \tilde{B}_i^n$. An analogous scheme has been constructed for the solution of the balance energy equation for the minority carrier system.

Although all coefficients of these difference schemes preserve the positiveness property ($\tilde{A}_i^j, \tilde{B}_i^j, \tilde{C}_i^j > 0$, with $j = n, p$), this fact cannot guarantee monotonicity of the constructed schemes. The sign of the functions near $(\mathcal{E}_n)_i$ ($(\mathcal{E}_p)_i$) in the expressions for the operators Λ_{T_n} (Λ_{T_p}) cannot be defined *a priori*, and in the general case it may change. On each time step and in each point of space x_i the conditions $n_i \geq 0$, $T_n \geq 1$ (and respectively $p_i \geq 0$, $T_p \geq 1$) cannot be guaranteed numerically in the general case. Our numerical experiments for a microwave diode (Section 5) confirm the conclusion that the above conditions for temperature may be violated.

The verification of the conditions of the theorem on monotonicity (see [3] and references therein) leads to the following requirements for the majority carrier system

$$(G_n)_i = -\mu_n [(T_n)_i] \varphi_{xx,i} - \mu_n [(T_n)_i] (\varphi_{x,i})^2 / (T_n)_i + ((T_n)_i - 1) / (\tau_\omega^n [(T_n)_i] (T_n)_i) + 1.5 / \tau_{i+1} \geq 0. \quad (4.14)$$

It is easy to show that this condition (as well as a similar condition for the minority carrier system) will be satisfied if on each temporal level we couple the time step with the strength of electric field by the inequality $\tau < 1.5 / (E^*)^2$. In the stationary case the monotonicity conditions will be satisfied under the stability conditions (4.3). Computational experiments support this conclusion.

5. Numerical Experiments

We applied the difference schemes discussed in Section 4 to a number of problems related to the non-equilibrium behaviour of electron-hole plasma of semiconductors. In particular, computational experiments have been performed for silicon $p^+ - n - n^+$ diode structures. Such devices are widely used as microwave switches in many industrial applications.

The dopant distribution in the semiconductor structure was chosen as in [3] (ranging from $N = -1.0 \times 10^{18}$ to 2.4×10^{19}). The comparison of computational results for the diode that works in the forward-biased regime showed that the process of heating/cooling of electron-hole plasma is not essential. We observed no more than 12% deviation of the distribution of temperature for majority and minority carriers from the reference temperature 300^0K (8% in the vicinity of $p - n$ junctions) when different voltages in the range from 0 to 0.8 V were applied.

The situation changes drastically for the same diode working in the reversed-biased regime. The results are shown on Figures 1 (for major carriers) and 2 (for minority



FIGURE 1



FIGURE 2

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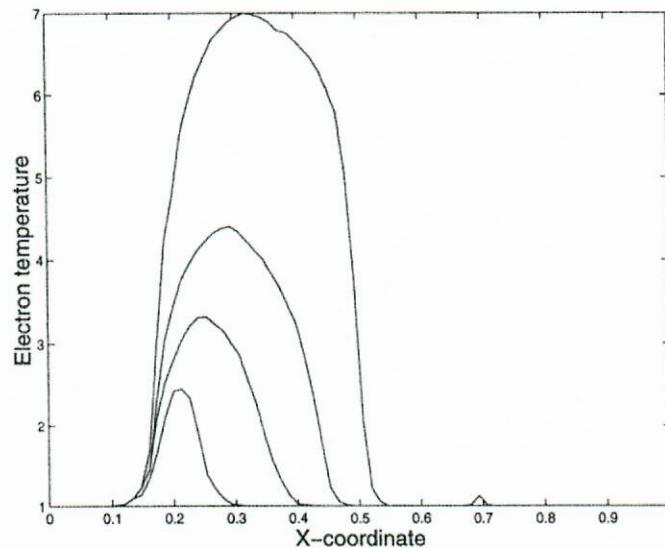


FIGURE 1. Electron temperature in the reversed-biased diode.

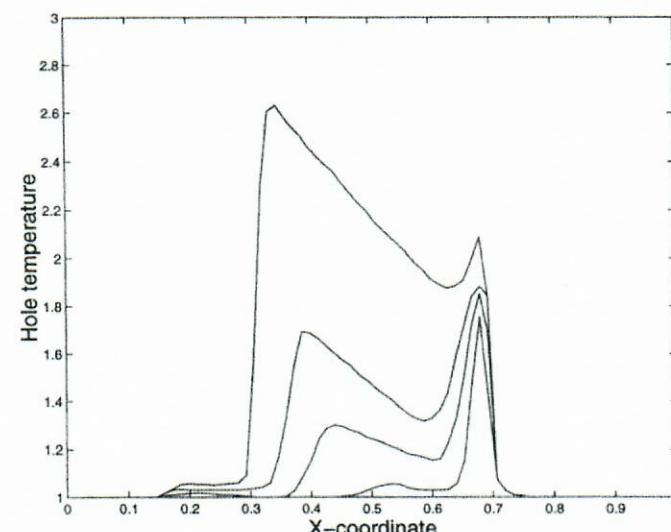


FIGURE 2. Hole temperature distribution in the reversed-biased diode.

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carriers) when $-0.5V$, $-1.0V$, $-1.5V$ and $-2.5V$ voltage were applied (curves are located respectively with a gradual increase in temperature). The observed "splash" of carrier velocities in the neighborhood of $p-n$ junction leads to a certain abating of their concentrations. In this case the coupling between electric field and effective temperature of carriers is non-local and the highest warming up takes place in the neighborhood of reverse-biased $p-n$ junctions. This effect cannot be observed using standard mathematical models of drift-diffusion type.

6. Conclusions and Future Directions

In this paper we analysed problems of mathematical modelling in microelectronics on the basis of a hierarchy constructed with respect to the relaxation time functions. For the investigation of non-equilibrium and non-local processes in semiconductors, effective numerical procedures based on non-conservative monotone schemes have been developed, algorithmic realization of the proposed schemes have been proposed and results of computational experiments on device modelling have been presented.

From the mathematical point of view the models considered in this paper provide an important practical example of stiff systems of partial differential equations with source terms. The availability of the conservative property for such systems depends on the definition of the source terms which are always the subject of approximations. If perturbation techniques are applied to such problems, the natural space for perturbations becomes L^1 rather than L^2 (see also [1, 4]). A challenging problem arises from the fact that the flow map representing the solution of such systems is typically not differentiable with respect to the linear structure of L^1 . This leads to major difficulties in the investigation of systems that are described by stiff PDEs, because the contractivity property of the flow for such systems with respect to L^1 -distance is no longer true in general. As a result, reasonable alternatives to classical and continuous models for semiconductor devices are discrete physical-topological models, semi-classical and quantum models. In the development of such models the role of effective computational techniques essentially increases.

7. Acknowledgements

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