Nonlinear Models for Silicon Semiconductors

Salvatore La Rosa, Giovanni Mascali, and Vittorio Romano

Abstract In this paper we present exact closures of the 8-moment and the 9-moment models for the charge transport in silicon semiconductors based on the maximum entropy principle. The validity of these models is assessed by numerical simulations of an n-$^+$n-n$^+$ device. The results are compared with those obtained from the numerical solution of the Boltzmann Transport Equation both by Monte Carlo method and directly by a finite difference scheme.

1 Introduction

Simulation of modern electronic devices requires increasingly accurate models of charge transport in semiconductors in order to describe high-field phenomena such as hot electron propagation, impact ionization and heat generation. Moreover, in many applications in optoelectronics, it is necessary to describe the transient interaction of electromagnetic radiation with carriers in complex semiconductor materials: in these cases the characteristic times are of the order of the electron momentum or the energy flux relaxation times. These are some of the main reasons of the necessity of developing models which incorporate a number of moments of the distribution function higher than those in the drift-diffusion and the energy transport models.

These extended models, generally called hydrodynamical models, are usually derived from the infinite hierarchy of the moment equations of the Boltzmann Transport Equation (BTE) by suitable truncation procedures. One of the most successful

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J. Roos and Luis R.J. Costa (eds.), *Scientific Computing in Electrical Engineering SCEE 2008*, Mathematics in Industry 14, DOI 10.1007/978-3-642-12294-1_53,

among these procedures is that based on the Maximum Entropy Principle (MEP) [1], see [2] for a complete review both for Si and GaAs semiconductors.

The models differ for the number of moments which are used and they usually comprise the balance equations of the electron density, the energy density, the average velocity, the energy flux and possibly also higher scalar and vector moments which do not have an immediate physical interpretation. In this paper we present the usual 8-moment model [3] together with a 9-moment model in which a further scalar moment is added: that corresponding to the squared microscopic electron energy. The two models are assessed by applying them to the benchmark problem of an n-$^+$n-n$^+$ silicon device.

2 Hydrodynamical Models with 8 and 9-Moments

In [3] we presented an 8-moment model for charge transport in semiconductors and we assessed its validity. In principle, one can try to improve this model by adding further scalar and vector moments as well as higher order tensor moments. Adding the scalar moment nW_2, one obtains a new model which is given by the following system of balance equations

$$\frac{\partial n}{\partial t} + \frac{\partial (nV^i)}{\partial x^i} = 0, \tag{1}$$

$$\frac{\partial (nV^i)}{\partial t} + \frac{\partial (nU^{ij})}{\partial x^j} + neE_j H^{ij} = nC_{V^i}, \tag{2}$$

$$\frac{\partial (nW)}{\partial t} + \frac{\partial (nS^i)}{\partial x^i} + neV_i E^i = nC_W, \tag{3}$$

$$\frac{\partial (nS^i)}{\partial t} + \frac{\partial (nF^{ij})}{\partial x^j} + neE_j G^{ij} = nC_{S^i}. \tag{4}$$

$$\frac{\partial (nW_2)}{\partial t} + \frac{\partial (nS_2^i)}{\partial x^i} + 2neE_i S^i = nC_{W_2}, \tag{5}$$

where e is the absolute value of the electron charge and $\mathbf{E}$ the electric field. The macroscopic quantities, which are involved in the balance equations, are related to the electron distribution function $f(\mathbf{x},\mathbf{k},t)$ by the definitions

$$n = \int_{\mathbb{R}^3} f \mathrm{d}\mathbf{k}, \quad \text{electron density},$$

$$W = \frac{1}{n}\int_{\mathbb{R}^3} \mathscr{E}(k) f \mathrm{d}\mathbf{k}, \quad \text{average electron energy},$$

$$W_2 = \frac{1}{n}\int_{\mathbb{R}^3} \mathscr{E}^2(k) f \mathrm{d}\mathbf{k}, \quad \text{average electron energy square},$$

$$
\begin{aligned}
V^i &= \frac{1}{n}\int_{\mathbb{R}^3} f v^i \mathrm{d}\mathbf{k}, \quad \text{average velocity},\\
S^i &= \frac{1}{n}\int_{\mathbb{R}^3} f v^i \mathscr{E}(k)\mathrm{d}\mathbf{k}, \quad \text{energy flux},\\
S_2^i &= \frac{1}{n}\int_{\mathbb{R}^3} f v^i \mathscr{E}^2(k)\mathrm{d}\mathbf{k}, \quad \text{flux of the electron energy square},\\
U^{ij} &= \frac{1}{n}\int_{\mathbb{R}^3} f v^i v^j \mathrm{d}\mathbf{k}, \quad \text{velocity flux},\\
H^{ij} &= \frac{1}{n}\int_{\mathbb{R}^3} \frac{1}{\hbar} f \frac{\partial}{\partial k_j}(v^i)\mathrm{d}\mathbf{k}, \quad \text{(no physical interpretation)},\\
F^{ij} &= \frac{1}{n}\int_{\mathbb{R}^3} f v^i v^j \mathscr{E}(k)\mathrm{d}\mathbf{k}, \quad \text{flux of the energy flux},\\
G^{ij} &= \frac{1}{n}\int_{\mathbb{R}^3} \frac{1}{\hbar} f \frac{\partial}{\partial k_j}(\mathscr{E} v^i)\mathrm{d}\mathbf{k}, \quad \text{(no physical interpretation)},
\end{aligned}
$$

$$
\begin{aligned}
C_{V^i} &= \frac{1}{n}\int_{\mathbb{R}^3} \mathscr{C}[f] v^i \mathrm{d}\mathbf{k}, \quad \text{velocity production},\\
C_W &= \frac{1}{n}\int_{\mathbb{R}^3} \mathscr{C}[f] \mathscr{E}(k)\mathrm{d}\mathbf{k}, \quad \text{energy production},\\
C_{S^i} &= \frac{1}{n}\int_{\mathbb{R}^3} \mathscr{C}[f] v^i \mathscr{E}(k)\mathrm{d}\mathbf{k}, \quad \text{energy flux production},\\
C_{W_2} &= \frac{1}{n}\int_{\mathbb{R}^3} \mathscr{C}[f] \mathscr{E}^2(k)\mathrm{d}\mathbf{k}, \quad \text{electron energy square production},
\end{aligned}
$$

here $\mathscr{E}$ and $\mathbf{k}$ respectively are the electron energy in the conduction band and the wave vector, and $\mathscr{C}[f]$ is the collision operator which appears at the left hand of the BTE. These equations are coupled to the Poisson equation for the electric potential ϕ

$$E^i = -\frac{\partial \phi}{\partial x_i}, \tag{6}$$

$$\nabla \cdot (\varepsilon \nabla \phi) = -e(N_+ - N_- - n), \tag{7}$$

where ε is the electric permittivity and N_+ and N_- are the donor and acceptor density respectively (which depend only on the position).

The system (1)–(5) is not closed since the fluxes $\mathbf{S}_2, U, H, F, G$ and the production terms $C_{\mathbf{V}}, C_W, C_{\mathbf{S}}, C_{W_2}$ have to be expressed as functions of the fundamental variables $n, \mathbf{V}, W, \mathbf{S}$ and W_2. The closure can be achieved by means of MEP, using the distribution function which maximizes missing information (entropy) in order to

evaluate the unknown moments. This distribution function is called the maximum entropy distribution function f_{ME} [1, 2]. The MEP approach leads to a constrained optimization problem which is handled by resorting to the Lagrangian multipliers method, see [2] and references therein. In the present case, the constraints consist of the known moments $n, \mathbf{V}, W, \mathbf{S}$ and W_2 and they are used to express the Lagrange multipliers in terms of these moments. Actually, this is a highly non-linear problem, which, in the past, has been solved by assuming the distribution function to be slightly anisotropic and expanding it with respect to a suitable anisotropy parameter [2]. Recently [3] this problem has been solved numerically without resorting to asymptotic procedures. In this way the model is expressed in terms of the Lagrangian multipliers and the constitutive relations are given by integral expressions that do not allow an efficient numerical tabulation, but require the use of suitable quadrature formulas with respect to the microscopic energy. The interested reader is referred to [3] for the closure relations relative to the 8-moment model, the relations referring to the further quantities appearing in (5) being completely analogous. At the end apart from the Poisson equation, the resulting system is hyperbolic in the physically relevant region of the field variables.

It is important to notice that in the numerical integration of the models problems can arise due to the fact that there may exist moments that are not moments of the maximum entropy distribution [4]. In fact the set of the moments generated by f_{ME} is a convex cone $\mathscr{M}$ [5]. In the 8-moment case $\mathscr{M}$ is generated by the Lagrangian multipliers such that

$$g(\lambda^W, \lambda^{\mathbf{S}}) = \lambda^W - \sqrt{\frac{1}{2\alpha m^*}} ||\lambda^{\mathbf{S}}|| > 0, \tag{8}$$

while in the 9-moment case the cone is generated by the Lagrangian multipliers which satisfy

$$\lambda^{W_2} > 0. \tag{9}$$

Here α is the non-parabolicity factor, m^* the electron effective mass, $\lambda^W, \lambda^{\mathbf{S}}$ and λ^{W_2} are the Lagrange multipliers which correspond to W, $\mathbf{S}$ and W_2, respectively. The conditions are obtained by requiring the integrability of f_{ME}.

3 Simulation of an n-$^+$n-n$^+$ Device

We have tested the 8 and 9-moment models by numerically solving them in the 1-D problem of an n-$^+$n-n$^+$ device, which is commonly used as a benchmark problem [6]. In this case the systems have the following form

$$\frac{\partial F^{(0)}(\Lambda)}{\partial t} + \frac{\partial F^{(1)}(\Lambda)}{\partial x} = G(\Lambda, E), \tag{10}$$

where Λ is the vector of the unknown Lagrange multipliers, $F^{(0)}$ is the vector of the moments, $F^{(1)}$ is the vector of the fluxes and G is the vector of the sources which takes into account both the effect of the scatterings that electrons suffer inside the device and the driving effect of the electric field. (10) is solved by using a splitting strategy, which consists of two successive steps [3]: the first step solves the system without sources (convection step), while the second step solves the system with the fluxes put equal to zero (relaxation step).

The convection step makes use of the Nessyahu–Tadmor scheme [7], which does not require the explicit knowledge of the characteristic structure of the system and is conservative and consistent. The latter two properties are necessary requirements for having correct shock capturing methods. The relaxation system is a system of ordinary differential equations, which can be solved by using an explicit Euler scheme.

The devices which have been considered are those reported in Table 1.

Table 1: L_c length of the channel, doping concentration (respectively in the n^+ and n regions) and V_b applied voltage

Channel length L_c (μm)	n^+ (10^{17} cm^{-3})	n (10^{17} cm^{-3})	V_b Volt
0.2	10	0.1	1
0.1	10	0.1	1

The results of the two non-linear models presented here (indicated by 8 and 9-moment NLMEP models respectively) have been compared with those obtained by the direct solution of the BTE (DSBE), with Monte Carlo results (MC) and also with those derived by means of the model in which the closure is based on the asymptotic expansion (indicated as SLMEP model) [8]. The aim is threefold:

- to check the validity of the 8 and 9 moment models,
- to assess the relevance of the nonlinearity,
- to see if the integrability condition is always satisfied.

As regards the validity, we can say that the results of the 8-moment model are satisfactory. In fact, as can be seen from Figures 1 and 2, which refer to devices with channel length equal to 0.2μm and 0.1μm respectively, the 8-moment NLMEP model gives the solutions closest to those obtained both with the MC method and the direct integration of the BTE. This means that the anisotropy effects are not small when the channel is short and there are high electric fields inside the device. The solutions do not show any spurious oscillations which indicates that the assumed boundary conditions are compatible with the solutions of the problem: we have used Dirichlet conditions on the density and Neumann conditions on the Lagrange multipliers corresponding to the remaining moments, which are the fundamental variables of the model. Furthermore we also notice that the peak in the velocity near the second junction almost disappears in accordance with MC and DSBE results.

As regards the integrability, the problem is subtle. In fact in the transient there are wide oscillations which can bring the numerical solution out of the cone $\mathscr{M}$. As can

be seen from Figure 3 left, for a device with a channel length of 0.2μm this can be tackled by improving the precision of the numerical integration with respect to the microscopic energy in the closure relations. The numerical integration is effected by using the Gauss–Legendre formula and passing from 140 nodes to 310 nodes in the microscopic energy interval $[0\,\mathrm{eV}, 1.6\,\mathrm{eV}]$ the integrability is recovered. The situation is different when the channel length is 0.1μm, in this case in fact there is a region near the first junction, see Figure 3 right, where the integrability does not improve even by increasing the number of nodes. The case of the 9-moment model is worse; in fact, as can be seen from Figure 4 right below we do not have integrability, independently on how precise the integration is. This is probably due to the fact that additional Lagrangian multipliers, associated to new moments corresponding to weight functions represented by powers of energy with an exponent greater than one, are zero at equilibrium states which are, therefore, located at the boundary of the realizability region. This implies that small perturbations can have both positive and negative sign causing a loss of integrability and limiting the validity of the non-linear models. As a consequence the solution of the 9-moment model, Figures 4_{1-3}, is clearly unreliable.

4 Conclusion

In conclusion, the results, which we have obtained, make us affirm that a great attention has to be payed to whether the integrability condition is satisfied when using a completely non-linear model. The problem could be effectively solved by using a better approximation for the energy bands, in which the Brillouin zone, instead of being extended to all $\mathbb{R}^3$ as for the Kane dispersion relation, is a limited region as in the physical case.

Acknowledgements The authors acknowledge the financial support by M.I.U.R. (PRIN 2007 *Equazioni cinetiche e idrodinamiche di sistemi collisionali e complessi*), P.R.A. University of Catania and University of Calabria (ex 60 %), CNR (grant n. 00.00128.ST74), the EU Marie Curie RTN project COMSON grant n. MRTN-CT-2005-019417.

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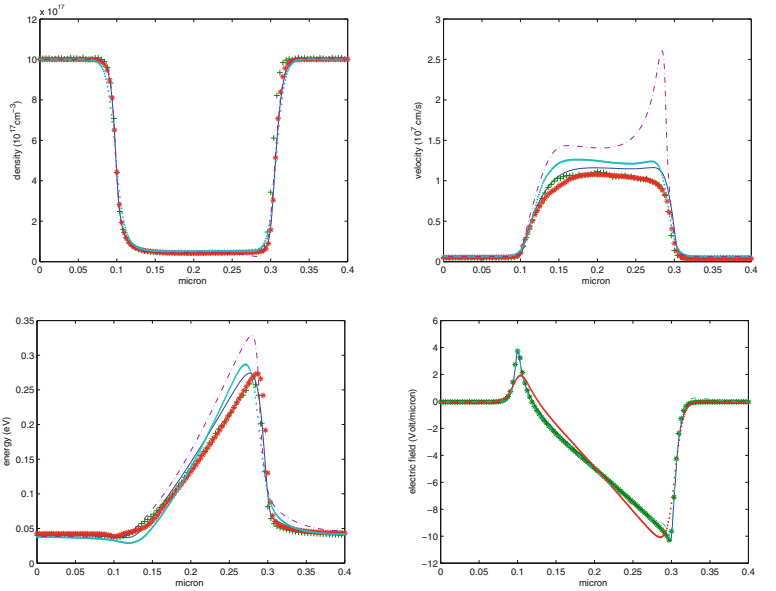

Fig. 1: $L_c = 0.2\ \mu$m, stationary solution: 8 moment-NLMEP model (*continuous line*), SLMEP model (*dotted line*), MC simulation (*crossed line*), direct Boltzmann integration (*starry line*) and Baccarani Blotekjaer Wordeman (BBW) model (*dashed-dotted line*)

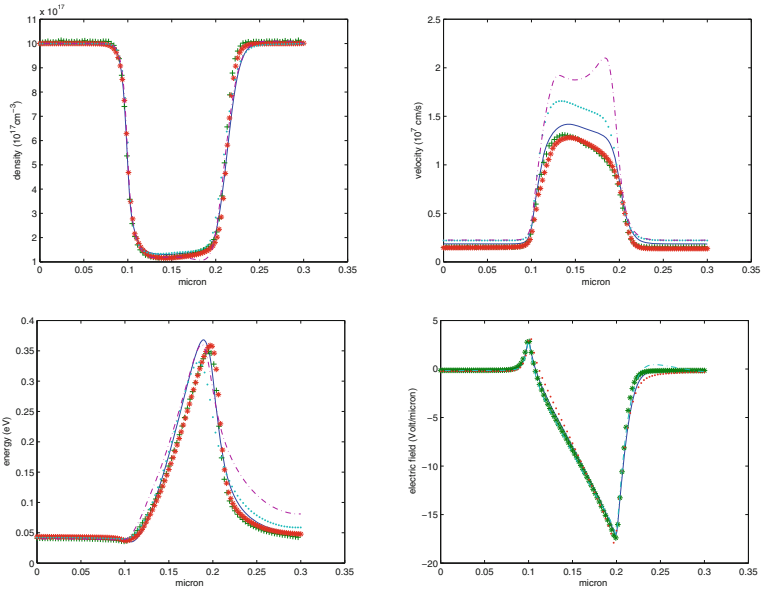

Fig. 2: $L_c = 0.1\ \mu$m, stationary solution: 8 moment-NLMEP model (*continuous line*), SLMEP model (*dotted line*), MC simulation (*crossed line*), direct Boltzmann integration (*starry line*) and BBW model (*dotted line*)

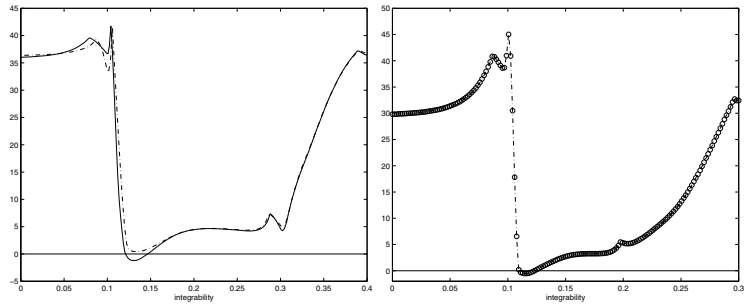

Fig. 3: $L_c = 0.2\,\text{and}\,0.1\,\mu\text{m}$, integrability condition. *Left*: 140 nodes in the energy interval (in eV) [0,1.55] (*continuous line*), 310 nodes in [0,1.6] (*dashed-dotted line*). *Right*: 490 nodes in [0,3.39] (*circles*), 735 nodes in [0,3.39] (*dashed-dotted line*)

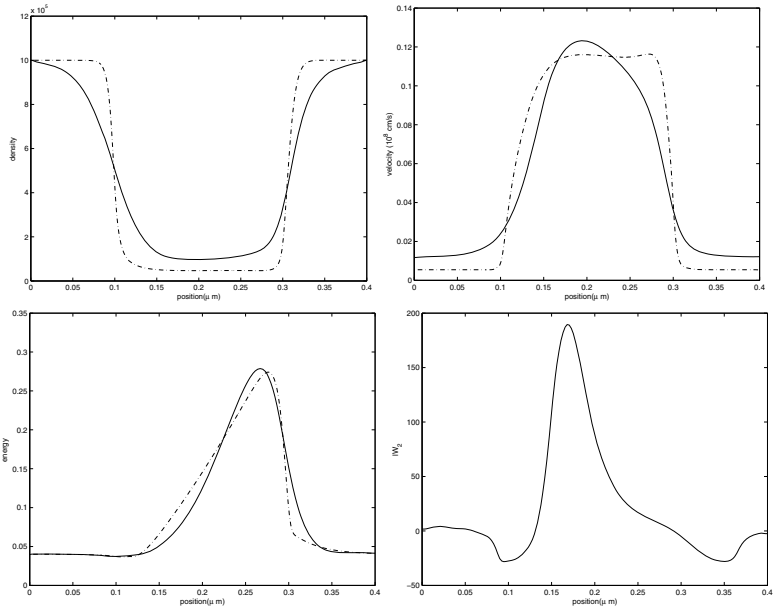

Fig. 4: $L_c = 0.2\ \mu\text{m}$, stationary solution: 8 moment-NLMEP model (*dashed-dotted line*), 9 moment-NLME model (*continuous line*). Integrability: plot of λ^{W_2} versus the position

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