NUMERICAL SIMULATION OF HIGH-FIELD TRANSPORT USING A FLUX-CORRECTED TRANSPORT ALGORITHM

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Abstract

Hydrodynamic simulations of high-field transport are performed using a flux-corrected transport algorithm. This efficient algorithm uses careful control of numerical diffusion to achieve high accuracy in simulating flow phenomena in the presence of steep gradients as can occur in small devices where overshoot phenomena are significant. We apply the flux-corrected transport scheme to a preliminary evaluation of various hydrodynamic descriptions of high-field transport.

I. INTRODUCTION

Continuum or hydrodynamic descriptions of electron transport have long been applied in the analysis and design of semiconductor devices because they provide a useful compromise between computational simplicity and physical fidelity. As devices continue to scale deep into the sub-micron regime such descriptions will continue to be of value although ultimately they must break down. The transport in deep submicron regimes is often characterized by high electric fields, rapidly varying densities and history-dependent phenomena (including inertia) which make the governing equations more hyperbolic in character. From a computational standpoint these factors and particularly the need to obtain accurate results in the vicinity of steep gradients represent significant challenges. One numerical approach capable of handling these difficulties which has been widely used for fluid simulation in other fields is flux-corrected transport (FCT) [1]. In essence, FCT is an explicit, spatially high-order finite-difference scheme in which a conservative "flux-limiting" procedure is used to prevent the otherwise inevitable unphysical ripples which would appear in the numerical solution near steep gradients. In this work, we apply an FCT algorithm to solving hydrodynamic equations describing electron transport in small-geometry n^+-n-n^+ silicon diodes.

In addition to studying the numerical issues, a primary purpose of our effort is to examine and give a preliminary evaluation of various hydrodynamic descriptions of high-field electron transport. Such descriptions are founded on a continuum approximation, i.e., that meaningful density variables can be defined, and in electron transport work are typically derived by taking velocity moments of the Boltzmann equation. Alternatively, hydrodynamic descriptions may be developed using classical field theory [2]. The former approach emphasizes the connections to the underlying microscopic physics whereas the latter, which takes the density variables as *primitives*, focuses on the consequences of general principles of balance, invariance and symmetry, i.e., on what is physically possible given a certain set of primitive densities. Obviously, the larger this set the more physics can be described at the expense of utility. In Sec. II we outline the equations which stem from standard choices for the density variables and then discuss numerical methods and solutions in Secs. III and IV.

II. HYDRODYNAMIC MODELS OF ELECTRON TRANSPORT

We consider describing the flow of the population of conduction band electrons through a semiconductor as the flow of a single fluid through a solid. The primitives of the theory are therefore the quantities which define this electron fluid and its interaction with itself, with the lattice and with the electrostatic field at every point. As a first case, we assume that the fluid is describable by the primitives of mass/charge density, momentum density and energy density. The laws of mass,

momentum and energy balance and of electrostatics then lead to a set of equations constraining these densities as follows [2]:

$$\text{(1a)}\quad n_{,t} + \nabla\cdot(n\mathbf{u}) = 0\ , \qquad mn\frac{d\mathbf{u}}{dt} = -\nabla p^n + \nabla\cdot\tau^n - qn(\mathbf{E}+\mathbf{E}^n)\ , \qquad \nabla\cdot\mathbf{D} = q(N_D - n)\ ,$$

$$\text{(1b)}\quad mn\frac{d\varepsilon^n}{dt} = -\nabla\cdot\mathbf{q}^n + \tau^n:\mathbf{d} + \frac{p^n}{n}\frac{dn}{dt} + qnE_d^n\cdot\mathbf{u} + mns^n, \qquad \rho\frac{\partial\varepsilon^l}{\partial t} = -\nabla\cdot\mathbf{q}^l + \mathbf{E}\cdot\frac{\partial P}{\partial t} + qnE_r^n\cdot\mathbf{u} + \rho s^l\ ,$$

where n, $\mathbf{u}$, $mn\varepsilon^n$, $\mathbf{q}^n$, mns^n are the number density, velocity, energy density, heat flux and energy source density of the electron gas, ρ, N_D, $\rho\varepsilon^l$, $\mathbf{q}^l$ and ρs^l are the mass density, ionized impurity density, energy density, heat flux and energy source density of the lattice, $\mathbf{E}_r^n$ and $\mathbf{E}_d^n$ are the recoverable and dissipative parts of the force (per charge) exerted by the lattice on the gas, p^n and τ^n are the electron gas pressure and viscous stress, $\mathbf{E}$ and $\mathbf{D}$ ($=\mathbf{P}+4\pi\mathbf{E}$) are the electric field and electric displacement, $\mathbf{d}$ is the rate-of-deformation tensor and d/dt is the material derivative.

The differential equations (1) represent a set of physical constraints on the density variables; they are not sufficient however to determine these densities. To make the system determinate constitutive equations specifying the material response must also be supplied. For example, the usual energy transport (ET) model [3] results if we select the following constitutive equations

$$\text{(2)}\quad p^n = kT^n n\ , \qquad \tau^n = 0\ , \qquad E_r^n = 0\ , \qquad E_d^n = \frac{\mathbf{u}}{\mu_{LF}}\frac{T^n}{T^l}\ ,$$

$$m\varepsilon^n = \frac{3}{2}kT^n\ , \qquad \mathbf{q}^n = -\frac{3}{2}D_{LF}nk\nabla T^n\ , \qquad mns^n = -\rho s^l = -\frac{n}{\tau_w}\left[\frac{m^*}{2}\mathbf{u}\cdot\mathbf{u} + \frac{3k}{2}(T^n - T^l)\right],$$

where m^* is the electron effective mass, T^n and T^l are electron and lattice temperatures, μ_{LF} and D_{LF} are the low-field mobility and diffusivity and τ_w is an energy relaxation time. Now, as discussed in Ref. 2, *when heat conduction is small* the density variables of mass and momentum become adequate to describe the system. In this case, the energy balance equations (1b) need not be solved and the governing equations become (1a) plus constitutive equations which in Ref. 2 were selected as

$$\text{(3a)}\quad p^n = kT^l n\ , \qquad \tau^n = \lambda_v I\nabla\cdot\mathbf{u} + 2\mu_v\mathbf{d}\ , \qquad E_r^n = -\chi\frac{d\mathbf{u}}{dt}\ , \qquad E_d^n = \frac{\mathbf{u}}{\mu}\ ,$$

where

$$\text{(3b)}\quad \mu = \frac{2\mu_{LF}}{1+\sqrt{1+\dfrac{\mu_{LF}\hat{E}}{\sqrt{2}u_{sat}} + 4\left(\dfrac{\mu_{LF}\hat{E}}{u_{sat}}\right)^2}}\ , \qquad \hat{E} \equiv \left|\mathbf{E} - \tau_r\frac{d\mathbf{E}}{dt}\right|\ ,$$

λ_v and μ_v are viscosity coefficients, χ [$\equiv(m^*-m)/q$] is a drag rate coefficient arising from Bragg reflection, u_{sat} is the saturation velocity and τ_r is a "scattering equilibration time". We note the important inclusion in these equations of i) viscous effects and ii) memory or rate effects in the scattering (including as the origin of effective mass). The mobility model in (3b) is that of Ref. 5 with a rate term introduced to represent the delay associated with scattering. This reduced set of *electrohydrodynamic (EHD) equations*, which may be regarded as a physically well-founded version of Thornber's augmented diffusion-drift description [4], has obvious computational advantages and will be explored in our simulations below.

III. FLUX-CORRECTED TRANSPORT

Flux-corrected transport (FCT) is a powerful numerical method for integrating generalized continuity equations [1] which has been widely used for fluid simulation in other fields but has not been applied heretofore to semiconductor transport problems. FCT is an explicit, spatially high-order finite-difference scheme which is especially effective at providing high-accuracy solutions in the vicinity of steep gradients without exhibiting the unphysical ripples often seen in conventional schemes as a result of numerical dispersion. It accomplishes this by carefully controlling the amount of numerical diffusion in the scheme using a conservative "flux-correction" procedure which preserves monotonicity with maximal accuracy. Explicitly, FCT first computes provisional values for

the density (of mass, momentum or energy) $\hat{\rho}_i^k$ at the next time step k at each mesh point i using a low-order, strongly-diffused scheme. It then improves the accuracy of these values by removing as much of the numerical diffusion as possible without generating new or accentuating existing extrema. This is done in a conservative manner via

$$\rho_i^k = \hat{\rho}_i^k - f_{i+1/2}^k + f_{i-1/2}^k , \tag{4a}$$

where

$$f_{i+1/2}^k = S\cdot\max\left\{0,\min\left[S\cdot\left(\hat{\rho}_{i+2}^k - \hat{\rho}_{i+1}^k\right), \mu_{i+1/2}\left(\hat{\rho}_{i+1}^k - \hat{\rho}_i^k\right), S\cdot\left(\hat{\rho}_i^k - \hat{\rho}_{i-1}^k\right)\right]\right\} \tag{4b}$$

is the corrected flux, $S \equiv \mathrm{sgn}\left(\hat{\rho}_{i+1}^k - \hat{\rho}_i^k\right)$ and $\mu_{i+1/2}$ is an antidiffusion coefficient chosen to minimize the residual numerical error [6]. That the corrections are functions of the solution means that the scheme is nonlinear. We note that the idea behind FCT has been incorporated in a number of other numerical schemes known collectively as nonlinear monotone methods. Among these are the essentially non-oscillatory (ENO) schemes [7] which have been applied to semiconductor transport problems [8]. All of these methods have similar advantages; we believe FCT to be preferred only because of its conceptual simplicity which enables, for example, straightforward generalization to more than one dimension [9]. In the calculations of this paper, FCT is used to solve the hydrodynamic equations and the electrostatics is solved conventionally in a Gummel iteration.

IV. SIMULATION RESULTS

As a test problem we model the standard n^+-n-n^+ diode with the geometry and doping levels chosen to match those of Refs. 10 and 11. A one-dimensional boundary value problem modeling this structure is readily formulated in the ET [(1) with (2)] and EHD [(1a) with (3)] descriptions. We first solve this problem using FCT in the familiar ET case. The calculated steady-state velocity profile for a 0.4μm diode biased at 1.5V is shown in Fig. 1 along with the electron temperature profile. These results are essentially the same as those obtained in Ref. 11 using an implicit scheme. The ET description exhibits velocity overshoot which is qualitatively reasonable apart from the well-known spurious peak seen near the anode. The origin of the latter has been widely discussed and is not of interest here. However, in one additional run (Fig. 1) we included viscosity [using τ^n of (3a)] in the ET simulation and found that the spurious peak largely disappears indicating that viscosity needs to be considered if the ET model is to be fully understood. In any event, our main point is that FCT provides an efficient scheme for performing conventional energy transport simulations.

We next apply FCT to solving the EHD equations. Considering the same problem as in Fig. 1, the qualitatively reasonable result shown in Fig. 2 is obtained. We note that the EHD simulation shows no evidence of the spurious peak seen in the ET simulation. In Fig. 2 we also give an

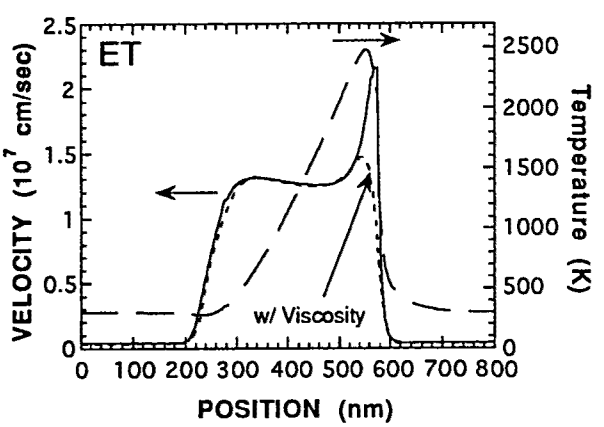

Fig. 1. ET velocity (with and without viscosity) and temperature profiles.

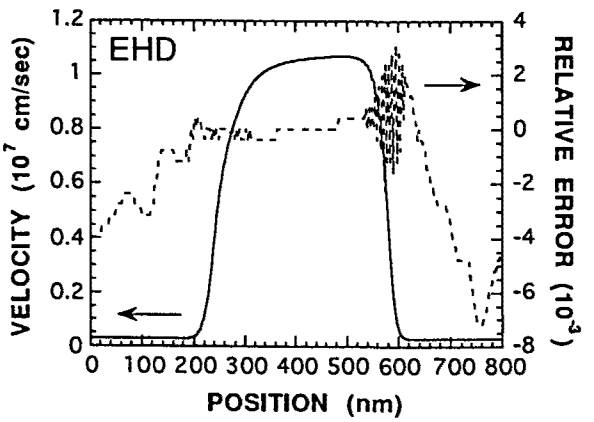

Fig. 2. Profiles of the EHD velocity and the relative error in the steady-state current.

indication of the numerical error introduced by the FCT scheme. We plot the deviations from uniformity in the steady state current as a relative error; the high accuracy possible with an FCT algorithm (here in single precision) is evident. Next, in Fig. 3 we compare the ET and EHD descriptions with profiles computed using diffusion-drift theory (DD) and by Monte Carlo solution of the Boltzmann equation (MC) [10]. This calculation is for a 0.1μm diode biased at 1V and the prediction of DD theory shows that the diode is operating in a strong velocity overshoot regime. In comparison with the "exact" MC solution, the EHD description is seen to do quite well both qualitatively and quantitatively. In this calculation, the one fitting parameter is the choice of τ_r to be 0.13psec. The ET description does significantly less well both in shape and magnitude, however, it should be said that no effort to adjust parameters such as the thermal conductivity has been made in the simulation. Finally, in Fig. 4 we exhibit the important roles of viscous and rate effects in the EHD description. The viscous effects smooth velocity gradients via dissipation, an effect which is partially offset by the rate effects which steepen the solution by delaying the onset of velocity saturation.

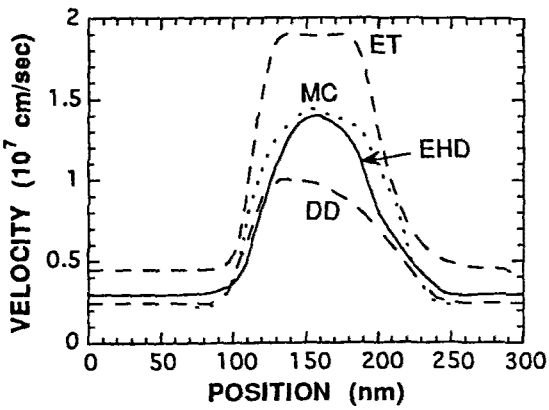

Fig. 3. Comparison of ET and EHD velocity profiles with diffusion-drift (DD) and Monte Carlo (MC).

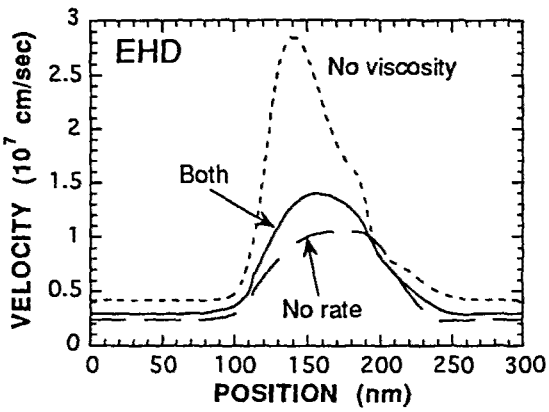

Fig. 4. EHD velocity profiles computed with and without mobility rate and viscous terms.

V. CONCLUSIONS

The main conclusion from this work is that the FCT algorithm provides a robust numerical approach to solving hydrodynamic equations descriptive of high field transport in semiconductors. It is a conceptually simple approach for which there exists a wide body of experience and software. It provides efficient, high accuracy solutions in the presence of steep gradients. and it is readily extendable to more than one space dimension. In this work, we applied this algorithm to the study of two high-energy transport theories. In the context of modeling overshoot phenomena, we find that an electrohydrodynamic description in which an energy balance equation is not solved gives accurate solutions with significant computational savings. Although these results are promising it is clear that more work is needed to fully validate this description and to determine its precise limitations.

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1. J.P. Boris and D.L. Book, *J. Comp. Phys.* **11**, 38 (1973).
2. M.G. Ancona, to be published, *VLSI Design* (1994).
3. K. Blotekjaer, *IEEE Trans. Elect. Dev.* **ED-17**, 38 (1970).
4. K.K. Thornber, *IEEE Elect. Dev. Lett.* **EDL-3**, 69 (1982).
5. D. Roychoudhury and P.K. Basu, *Solid-St. Electron.* **19**, 656 (1976).
6. J.P. Boris and D.L. Book, in *Methods in Comp. Phys.* **16**, Academic, New York, p. 85 (1976).
7. A. Harten and S. Osher, *SIAM J. Numer. Anal.* **24**, 279 (1987).
8. E. Fatemi, J. Jerome and S. Osher, *IEEE Trans. Comp.-Aided Design* **CAD-10**, 232 (1991).
9. S.T. Zalesak, *J. Comp. Phys.* **31**, 335 (1979).
10. E.C. Kan, U. Ravaioli and T. Kerkhoven, *Solid-St. Electron* **34**, 995 (1991).
11. C.L. Gardner, J. Jerome and D. Rose, *IEEE Trans. Comp.-Aided Design* **CAD-8**, 501 (1989).