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Simulation of a Steady-State Electron Shock Wave in a Submicron Semiconductor Device Using High-Order Upwind Methods

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Abstract

The hydrodynamic model treats electron flow in a semiconductor device through the Euler equations of gas dynamics, with the addition of a heat conduction term. Thus the hydrodynamic model PDEs have hyperbolic, parabolic, and elliptic modes.

The nonlinear hyperbolic modes support shock waves. Numerical simulations of a steady-state electron shock wave in a semiconductor device are presented, using steady-state second upwind and high-order time-dependent upwind methods. For the ballistic diode (which models the channel of a MOSFET), the shock wave is fully developed in Si (with a 1 volt bias) at 300 K for a 0.1 micron channel and at 77 K for a 1.0 micron channel.

1 Introduction

The hydrodynamic model equations consist of a set of nonlinear conservation laws for particle number, momentum, and energy, coupled to Poisson's equation for the electric potential. The nonlinear conservation laws are just the Euler equations of gas dynamics for a gas of charged particles in an electric field, with the addition of a heat conduction term [1]. Thus the hydrodynamic model PDEs have hyperbolic, parabolic, and elliptic modes.

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The nonlinear hyperbolic modes support shock waves. Electron shock waves should occur in silicon devices at short length scales or at low temperatures. Steady-state second upwind and high-order time-dependent upwind simulations of a steady-state electron shock wave in a semiconductor device will be presented, using the hydrodynamic model. The simulations were performed for the ballistic diode (which models the channel of a MOSFET). With a 1 volt bias across the diode, the shock wave is fully developed in Si at 300 K for a 0.1 micron channel and at 77 K for a 1.0 micron channel [2].

2 The hydrodynamic model

A fairly general set of transport equations for device simulation has been derived by Bløtekjær [3] from the Boltzmann equation:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0 \quad (1)$$

$$\frac{\partial \mathbf{p}}{\partial t} + \mathbf{v} \nabla \cdot \mathbf{p} + \mathbf{p} \cdot \nabla \mathbf{v} = -en\mathbf{E} - \nabla(nT) + \left(\frac{\partial \mathbf{p}}{\partial t} \right)_c \quad (2)$$

$$\frac{\partial W}{\partial t} + \nabla \cdot (\mathbf{v}W) = -en\mathbf{v} \cdot \mathbf{E} - \nabla \cdot (\mathbf{v}nT) + \nabla \cdot (\kappa \nabla T) + \left(\frac{\partial W}{\partial t} \right)_c \quad (3)$$

where n is the electron density, \mathbf{v} is the velocity, \mathbf{p} is the momentum density, e (> 0) is the electronic charge, \mathbf{E} is the electric field, T is the temperature in energy units, W is the energy density, κ is the heat conduction coefficient, and the subscript c indicates collision terms. We will assume that the energy bands are parabolic:

$$\mathbf{p} = mn\mathbf{v}, \quad W = \frac{3}{2}nT + \frac{1}{2}mnv^2 \quad (4)$$

where m is the effective electron mass.

In addition to the transport equations (1)–(3), we have Poisson's equation for the electric field

$$\nabla \cdot (\epsilon \nabla \phi) = -e(N_D - N_A - n), \quad \mathbf{E} = -\nabla \phi \quad (5)$$

where N_D is the density of donors and N_A is the density of acceptors. Eqs. (1)–(5) determine the variables n , \mathbf{p} , W , and ϕ .

Eqs. (1)–(3) are in conservation form, and may be written in terms of the variables n , \mathbf{v} , T , and ϕ . These variables represent the simplest choice for upwind methods and for the ballistic diode boundary conditions.

3 The ballistic diode problem

As a model problem, we simulate the flow of electrons in a submicron $n^+ - n - n^+$ silicon diode. This device models the channel in a MOSFET, and clearly

exhibits hot carrier effects at submicron scales. The diode begins with an n^+ “source” region, is followed by an n “channel” region, and ends with an n^+ “drain” region.

Following Baccarani and Wordeman [4], we take

$$\left(\frac{\partial p}{\partial t}\right)_c = \frac{-P}{\tau_p}, \quad \tau_p = m \frac{\mu_{n0} T_0}{e T} \quad (6)$$

$$\left(\frac{\partial W}{\partial t}\right)_c = \frac{-(W - \frac{3}{2}nT_0)}{\tau_w}, \quad \tau_w = \frac{m \mu_{n0} T_0}{2 e T} + \frac{3 \mu_{n0} T T_0}{2 e v_s^2 T + T_0} \quad (7)$$

$$\kappa = \kappa_0 \frac{\mu_{n0}}{e} n T_0 \quad (8)$$

where T_0 is the ambient temperature, $\mu_{n0} = \mu_{n0}(T_0, N_D + N_A)$ is the low field electron mobility, and $v_s = v_s(T_0)$ is the saturation velocity.

The simplest boundary conditions for the simulations are $n = N$ and $T = T_0$ at x_{min} and x_{max} , and $e\phi(x_{min}) = T \ln(n/n_i)$ and $e\phi(x_{max}) = T \ln(n/n_i) + eV$, where V is the bias across the diode and n_i is the intrinsic electron concentration.

The steady-state computations use the second upwind method [2], a conservative discretization which captures the essential physical transport property of supersonic flow, that advected quantities directly influence the solution only downstream. We use Newton’s method to linearize the discretized steady-state hydrodynamic equations. Newton’s equation may be solved directly by sparse matrix techniques, or by block iterative methods [5].

The time-dependent simulations use an “essentially non-oscillatory” (ENO) upwind scheme [6]. The ENO method uses an approximate Riemann solver to evolve the solution preceded by an adaptive non-oscillatory reconstruction of the solution, and is capable of resolving shocks over 2-3 grid points. The upwind stencil is chosen to minimize the likelihood of crossing a discontinuity. The scheme we used is sixth-order accurate in space in regions of smooth flow.

4 Computations for transonic flow

Higher electron velocities can be obtained in a semiconductor device by making the active device length shorter. Since the electron soundspeed $c = \sqrt{T/m}$, higher electron Mach numbers may also be obtained by lowering the ambient temperature T_0 .

We present two parameter regimes for the ballistic diode in which there is a transition from subsonic to supersonic electron flow just to the right of the $n^+ - n$ junction and from supersonic to subsonic flow to the left of the $n - n^+$ junction. In analogy with gas dynamical flow in a Laval nozzle, a shock wave develops at the transition from supersonic to subsonic flow. The $n^+ - n - n^+$ doping of the ballistic diode corresponds to the converging-diverging geometry of the Laval nozzle. For further analysis of the shock waves, see Ref. [2].

For the transonic computations at $T_0 = 300$ K, we take a diode consisting of a 0.1 micron source, a 0.1 micron channel, and a 0.1 micron drain. In the n^+ region, the doping density $N = 5 \times 10^{17} \text{ cm}^{-3}$, while in the n region $N = 2 \times 10^{15} \text{ cm}^{-3}$.

Figs. 1 and 2 present a simulation of a Mach 1.6 electron shock wave at $V = 1$ volt (with 120 grid intervals) using the two upwind methods. The shock profile develops at $x_s \approx 0.035$ microns. The electron flow is subsonic behind the shock profile and supersonic ahead of the shock profile. The electron temperature is elevated well into the drain.

For the transonic computations at $T_0 = 77$ K, we take a diode consisting of a 0.1 micron source, a 1.0 micron channel, and a 0.1 micron drain. In the n^+ region, the doping density $N = 10^{18} \text{ cm}^{-3}$, while in the n region $N = 10^{15} \text{ cm}^{-3}$.

Figs. 3 and 4 present a simulation of a Mach 3.9 electron shock wave at $V = 1$ volt (with 120 grid intervals). Note the dramatic cooling of the electron gas as the electrons enter the channel, due to the potential barrier at the junction. The shock profile develops at $x_s \approx 0.3$ microns. Note that the shock wave is a much sharper profile in v and M than the Mach 1.6 shock wave. The high-order non-oscillatory scheme resolves the shock more sharply than the second upwind method, and will be important in resolving strong shocks and two-dimensional shocks.

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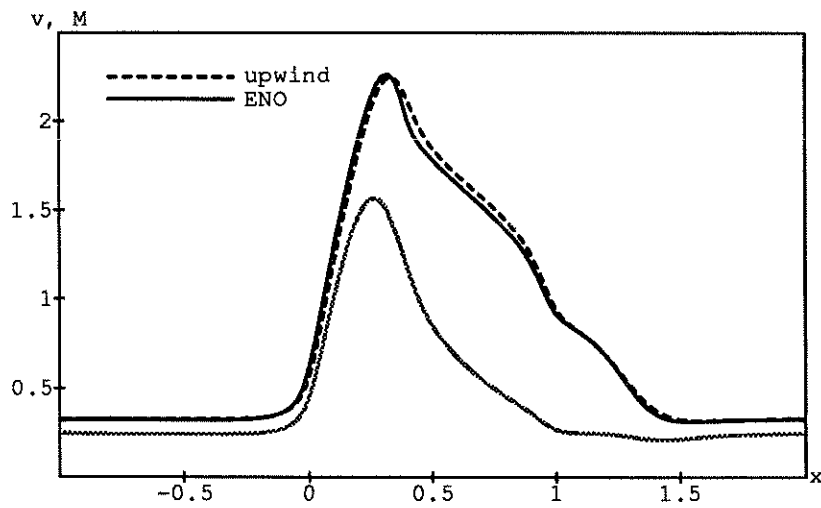


Figure 1: Electron velocity in 10^7 cm/s and electron Mach number (gray) for $V = 1$ volt, 0.1 micron channel, 300 K. x is in 0.1 microns.

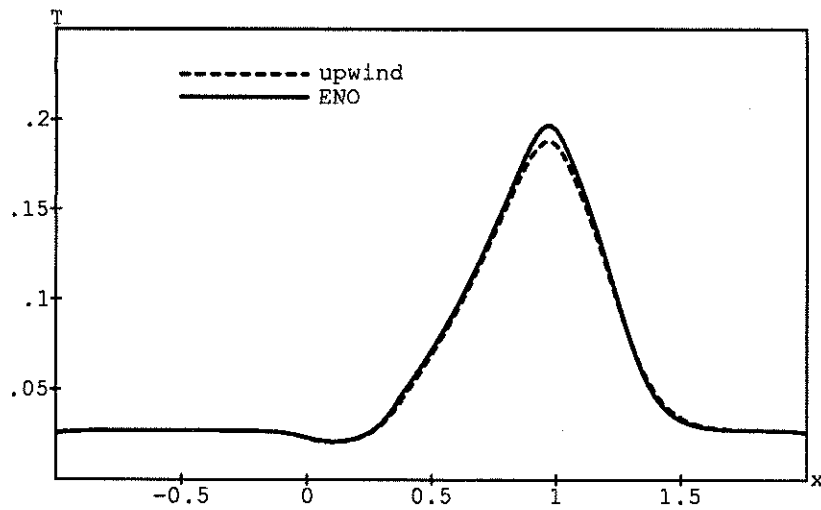


Figure 2: Electron temperature in eV for $V = 1$ volt, 0.1 micron channel, 300 K. x is in 0.1 microns.

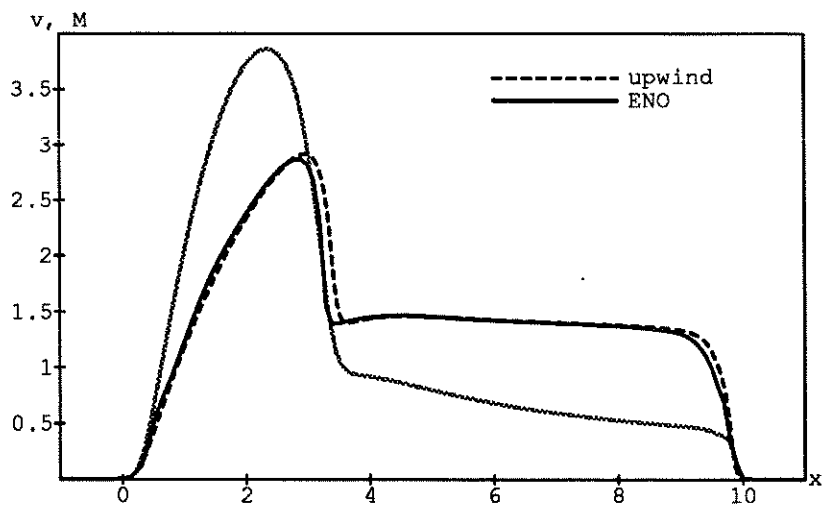


Figure 3: Electron velocity in 10^7 cm/s and electron Mach number (gray) for $V = 1$ volt, 1 micron channel, 77 K. x is in 0.1 microns.

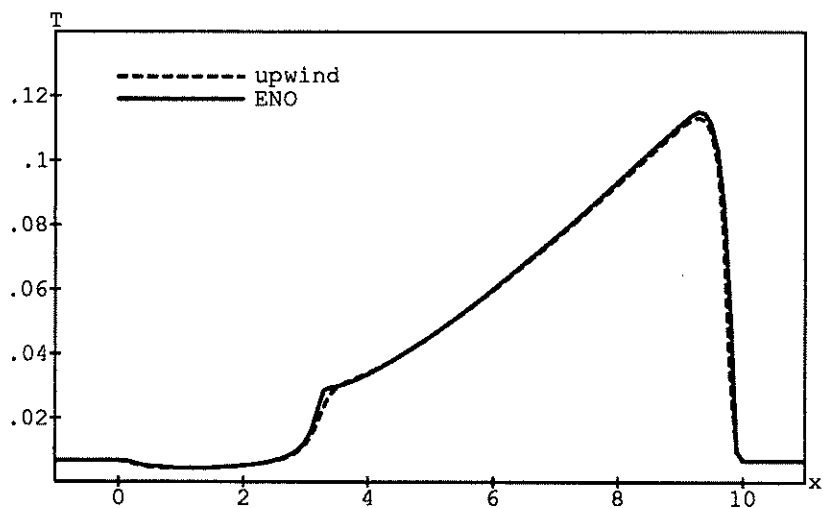


Figure 4: Electron temperature in eV for $V = 1$ volt, 1 micron channel, 77 K. x is in 0.1 microns.