Electron Vortices in Semiconductor Devices

Kamran Mohseni*, Ali Shakouri** and Rajeev J. Ram***

* Division of Engineering and Applied Sciences, 104-44 California Institute of Technology, mohseni@green.caltech.edu

** Jack Baskin School of Engineering, University of California, Santa Cruz, ali@cse.ucsc.edu

*** Department of Electrical Engineering, Massachusetts Institute of Technology, rajeev@mit.edu

ABSTRACT

The hydrodynamic model of electron transport in semiconductors is analyzed and in analogy to fluid mechanics the transport equation for the electron vorticity, $\nabla \times \mathbf{v}$, is derived. Aside from the classical hydrodynamic sources of vorticity, collision terms in the continuity and momentum equations may also generate electron vorticity. A scale analysis of the electron vorticity equation is performed and the relative order of magnitude of each source of vorticity is found. These analysis predict conditions for the observation of electron vortices in semiconductor devices.

Keywords: Electron vortices, electron transport, hydrodynamic model, submicron devices, semiconductors, scale analysis.

1 Introduction

As feature sizes in electronic devices get smaller and their speed increases we are entering in new regimes of electron transport in which traditional drift-diffusion models (cf. [1–4]) are not valid. While the drift-diffusion model provides a simple approach for large systems it fails to captures some of the important features of the electron transport in submicron systems. There has been extensive research to include quantum mechanical effects where wave nature of electrons plays an important role in the device operation. There has also been significant research on Monte Carlo methods [5, 6] to study the solutions of the Boltzmann transport equation and to consider effects such as velocity overshoot [7] and improved modeling of heat generation in the device [8,9]. While Monte Carlo simulations provide a direct numerical solution to the Boltzmann equation, costly computations make their practical usage limited. Another approach is to derive conservation laws for carrier density, momentum and energy by taking the moments of the Boltzmann equations, the so-called hydrodynamic models (e.g., see Blotekjaer [10] and Rudan and Odeh [11] and references therein). Apart from cheaper computational cost of these models (cf. [12]), their similarity to flow of compressible fluids provide almost an unlimited supply of theoretical and computational tools. The existence of shock fronts within the electron flow has been predicted by Gardner [13] using the hydrodynamic models. His simulations with a 1-V bias across the channel predicts fully developed shock waves at 300 K for a $0.1-\mu \mathrm{m}$ channel length and at 77 K for a $1.0-\mu \mathrm{m}$ channel length. de Jong and Molenkamp [14]have observed hydrodynamic Knudsen and Poiseuille flow of electrons in $4\mu \mathrm{m}$ wide wires at a temperature of $1.5\mathrm{K}$

In this paper we will analyze the problem of electron transport in ultra small devices from a hydrodynamic point of view. In the next section we consider the governing equations for electron transport in submicron devices. We systematically derive the electron vorticity transport equation in section 3, where similarities and differences with vorticity equation in fluids are clarified. In section 4 we perform a scale and order of magnitude analysis on the electron vorticity equation to obtain the relative importance of each source term in various transport regimes. Concluding remarks are given in section 5.

2 Governing equations

The Boltzmann transport equation for electrons moving with the group velocity ${\bf u}$ in an electric field ${\bf E}$ can be represented as

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{x}} f - \frac{e}{m} \mathbf{E} \cdot \nabla_{\mathbf{u}} f = C, \tag{1}$$

where e is the electron charge, m is the effective electron mass, C is the Collision term, $f(\mathbf{x}, \mathbf{u}, t)$ is the distribution function for the electrons, \mathbf{x} is the space variable, and t is time.

The first five moments in the velocity space are the balance equations for the flux of electron, momentum, and energy. These equations are represented as follows:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = C_n,\tag{2}$$

$$\frac{\partial \mathbf{p}}{\partial t} + \mathbf{v}(\nabla \cdot \mathbf{p}) + (\mathbf{p} \cdot \nabla)\mathbf{v} = -en\mathbf{E} - \nabla \cdot \mathbf{P} + \mathbf{C}_{\mathbf{p}}, \quad (3)$$

$$m\frac{\partial}{\partial t} \left(n \left[\frac{1}{2} |\mathbf{v}|^2 + e_I \right] \right) + m\nabla \cdot \left(\mathbf{v} n \left[\frac{1}{2} |\mathbf{v}|^2 + e_I \right] \right) + \nabla \cdot (\mathbf{v} \mathbf{P}) = -e n \mathbf{v} \cdot \mathbf{E} - \nabla \cdot \mathbf{q} + C_W. \tag{4}$$

Here, n is the electron concentration, \mathbf{v} is the translational velocity, \mathbf{p} is the momentum density $mn\mathbf{v}$, \mathbf{P} is the pressure tensor, \mathbf{q} is the heat flux, e_I is the internal energy, and C_n , $\mathbf{C_p}$, and C_W represent moments of C. These equations are supplemented by the Poisson equation for the electric potential ϕ

$$\mathbf{E} = -\nabla \phi, \tag{5}$$

$$\nabla \cdot (\epsilon \nabla \phi) = -\sum e_i n_i - k_1, \tag{6}$$

where $k_1 := \text{doping and } \epsilon := \text{dielectric.}$

3 Electron vorticity transport equation

Here we follow the approach used in the fluid dynamic community (e.g., see Batchelor [15]) to derive an equation for electron vorticity transport. Using the electron conservation equation (2) one can get the identity

$$\frac{\partial \mathbf{p}}{\partial t} + \mathbf{v}(\nabla \cdot \mathbf{p}) + (\mathbf{p} \cdot \nabla)\mathbf{v} :=
\frac{D\mathbf{p}}{\partial t} + \mathbf{p}\nabla \cdot \mathbf{v} = mn\frac{D\mathbf{v}}{Dt} + mC_n\mathbf{v},$$
(7)

where

$$\frac{D}{Dt} := \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla, \tag{8}$$

is the total derivative. Therefore the momentum equation (3) can be written as

$$\frac{D\mathbf{v}}{Dt} = -\frac{e}{m}\mathbf{E} - \frac{1}{mn}\nabla \cdot \mathbf{P} + \frac{1}{mn}\left(\mathbf{C}_{\mathbf{p}} - mC_n\mathbf{v}\right). \quad (9)$$

To obtain the vorticity equation we need to take the curl of the momentum equation (9). In doing so we need to calculate the curl of the acceleration term $D\mathbf{v}/Dt$. Using the vector identity

$$(\mathbf{v} \cdot \nabla)\mathbf{v} = \frac{1}{2}\nabla(\mathbf{v} \cdot \mathbf{v}) - \mathbf{v} \times (\nabla \times \mathbf{v}).$$

where $\nabla \times \mathbf{v}$ is the vorticity vector $\vec{\omega}$ we can write

$$\nabla \times \frac{D\mathbf{v}}{Dt} = \frac{\partial \vec{\omega}}{\partial t} - \nabla \times (\mathbf{v} \times \vec{\omega}). \tag{10}$$

Using the vector identity

$$\nabla \times (\mathbf{v} \times \vec{\omega}) = -(\mathbf{v} \cdot \nabla)\vec{\omega} + \mathbf{v}(\nabla \cdot \vec{\omega}) - \vec{\omega}(\nabla \cdot \mathbf{v}) + (\vec{\omega} \cdot \nabla)\mathbf{v},$$

the fact that the vorticity is a solenoidal vector field, and substituting $\nabla \cdot \mathbf{v}$ from the electron conservation equation (2) we obtain

$$\nabla \times (\mathbf{v} \times \vec{\omega}) = -(\mathbf{v} \cdot \nabla)\vec{\omega} - \left(C_n - \frac{Dn}{Dt}\right)\frac{\vec{\omega}}{n} + (\vec{\omega} \cdot \nabla)\mathbf{v}.$$
 (11)

Substituting equation (11) in equation (10) to get

$$\nabla \times \frac{D\mathbf{v}}{Dt} = n \frac{D}{Dt} \left(\frac{\vec{\omega}}{n} \right) + \frac{C_n}{n} \vec{\omega} - (\vec{\omega} \cdot \nabla) \mathbf{v}. \tag{12}$$

This is in fact the modified Beltrami vorticity equation [16] that includes sources of mass. Noting that $\nabla \times E = 0$, we can calculate the curl of the momentum equation (9) to obtain

$$n\frac{D}{Dt}\left(\frac{\vec{\omega}}{n}\right) - (\vec{\omega} \cdot \nabla)\mathbf{v} = -\nabla \times \left(\frac{1}{mn}\nabla \cdot \mathbf{P}\right) + \nabla \times \left(\frac{1}{mn}\left(\mathbf{C}_{\mathbf{p}} - mC_{n}\mathbf{v}\right)\right) - \frac{C_{n}}{n}\vec{\omega}.$$
 (13)

The collision terms are modeled as

$$C_n = -R, (14)$$

$$\mathbf{C_p} = -\frac{\mathbf{p}}{\tau},\tag{15}$$

$$C_W = -\frac{W - W_0}{\tau_w},$$
 (16)

where R is the recombination rate and τ_p and τ_w are the momentum and energy relaxation times, respectively. Therefore

$$n\frac{D}{Dt}\left(\frac{\vec{\omega}}{n}\right) - (\vec{\omega} \cdot \nabla)\mathbf{v} = -\nabla \times \left(\frac{1}{mn}\nabla \cdot \mathbf{P}\right) + \left(2\frac{R}{n} - \frac{1}{\tau_p}\right)\vec{\omega} + R\nabla\left(\frac{1}{n}\right) \times \mathbf{v}.$$
 (17)

Now we need a constitutional law (moment closure) for the pressure tensor \mathbf{P} . For simplicity, we consider an inviscid model, where we assume that the pressure tensor can be represented in terms of the effective carrier temperature T by an ideal gas law relationship

$$\mathbf{P} = nkT\mathbf{I},\tag{18}$$

Here I is the identity tensor and k is the Boltzmann constant. Therefore the vorticity equation (17) can be

written as

$$n\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla\right) \left(\frac{\vec{\omega}}{n}\right) = (\vec{\omega} \cdot \nabla)\mathbf{v} - \frac{k}{m} \nabla\left(\frac{T}{n}\right) \times \nabla n + \left(2\frac{R}{n} - \frac{1}{\tau_p}\right) \vec{\omega} + R \nabla\left(\frac{1}{n}\right) \times \mathbf{v}.$$
(19)

This is the electron vorticity transport equation. Note that since this is an inviscid model there is no vorticity redistribution due to diffusion. The main advantage of this equation over the classical hydrodynamic models of electron transport is that the electric field does not appear explicitly in the electron transport equation. This is due to the fact that electric fields are curl free.

There are seven terms involved in the vorticity equation (19). This equation shows that the ratio of the electron vorticity to the electron concentration can change with time due to the terms on the right-hand side of equation (19). The two terms on the left hand side form the total derivative of the vorticity density. The third term represents the vortex stretching essential for turbulence. The fourth term is similar to the baroclinic generation of vorticity in classical fluid mechanics and is due to the interaction of the principal part of the pressure tensor $\bf P$ and the density field n. The last three terms in equation (19) are due to vorticity generation through the collision terms in the continuity and momentum equations.

It is clear that in various regimes of electron transport, different terms in the electron vorticity equation are dominant. In large systems and under normal field conditions the vorticity sink term due to the interaction of vortices with the lattice damps out most of the electron vorticity generation. In the next section we perform an order of magnitude analysis to predict transport regimes in which electron vorticity dynamics play an important role.

4 Scaling and order of magnitude analysis

Since size and strength of the electric field applied to the device can vary significantly, it is interesting to compare the order of each term in the vorticity equation. We assume that the characteristic scales of the problem ie, velocity, length, electron concentration, temperature and electric field are given by U, L, n_0, T_0, E_0 , respectively. Note that the time scale is given by $\tau = L/U$ (for transport equations that includes source terms this scaling must be checked later). We can now introduce non-dimensional variables (assuming that the scaling is

the same in each direction)

$$\mathbf{x}^* = \frac{\mathbf{x}}{L}, \quad \mathbf{v}^* = \frac{\mathbf{v}}{U}, \quad t^* = \frac{U}{L}t, \quad n^* = \frac{n}{n_0}, \quad (20)$$

$$\vec{\omega}^* = \frac{L}{U}, \omega \quad T^* = \frac{T}{T_0}, \quad \mathbf{E}^* = \frac{\mathbf{E}}{E_0}, \quad \nabla^* = \frac{\nabla}{L}.$$
 (21)

Therefore, using the new variables, the vorticity equation will become

$$n^* \left(\frac{\partial}{\partial t^*} + \mathbf{v} \cdot \nabla^* \right) \left(\frac{\vec{\omega}^*}{n^*} \right) =$$

$$(\vec{\omega}^* \cdot \nabla^*) \mathbf{v}^* - \frac{kT_0}{mU^2} \nabla^* \left(\frac{T^*}{n^*} \right) \times \nabla^* n^* +$$

$$2 \frac{RL}{Un_0} \frac{\vec{\omega}^*}{n^*} - \frac{L}{U\tau_n} \vec{\omega}^* + \frac{RL}{Un_0} \nabla^* \left(\frac{1}{n^*} \right) \times \mathbf{v}^*. \tag{22}$$

In this equation one needs to find the appropriate scaling for T_0 and E_0 . The scaling for E_0 can be easily obtained from (5)

$$E_0 = \frac{\phi_0}{L_d},\tag{23}$$

where ϕ_0 is the scaling for the electric potential applied to the device. The scaling for T_0 may be obtained from the energy equation (4). In doing so we assume that the order of the main driving term $en\mathbf{v} \cdot \mathbf{E}$ is the same as the convective derivative on the left hand side. Of course after such assumption one should check its validity at the end of the calculations. Hence

$$T_0 = \frac{e\phi_0}{k} \tag{24}$$

It is important to note that even though the electric field does not enter directly in the vorticity equation, it sets the scaling for electron temperature in the device. Now we can write again the nondimensional vorticity equation with the appropriate scalings

$$n^* \left(\frac{\partial}{\partial t^*} + \mathbf{v} \cdot \nabla^* \right) \left(\frac{\vec{\omega}^*}{n^*} \right) =$$

$$(\vec{\omega}^* \cdot \nabla^*) \mathbf{v}^* - \frac{e\phi_0}{mU^2} \nabla^* \left(\frac{T^*}{n^*} \right) \times \nabla^* n^*$$

$$+ 2 \frac{RL}{Un_0} \frac{\vec{\omega}^*}{n^*} - \frac{L}{U\tau_p} \vec{\omega}^* + \frac{RL}{Un_0} \nabla^* \left(\frac{1}{n^*} \right) \times \mathbf{v}^*. \quad (25)$$

The three nondimensional numbers that appear on the right hand side of equation (25) are of fundamental importance in our analysis. The nondimensional number $e\phi_0/mU^2$ of the baroclinic term is the ratio of the absorbed energy of a free electron from the external potential ϕ_0 to the average thermal energy of electrons. The nondimensional number $L/U\tau_p = \tau/\tau_p$ in front of the momentum relaxation source term is in fact the ratio of the transit time to the momentum relaxation time. Note that the recombination rate can be represented

as $R \approx n_0/\tau_r$. Therefore, the nondimensional number $RL/Un_0 = L/U\tau_r = \tau/\tau_r$ in front of the recombination term in equation (25) can be interpreted as the ratio of the transit time in the device by the recombination relaxation time.

Since the momentum relaxation term acts as a sink of electron vorticity, we expect to be able to observe transport of electron vortices in regimes in which this term is smaller than the other source terms.

5 Conclusions

We analyzed the hydrodynamic model of electron transport in semiconductors and in analogy to fluid mechanics the transport equation for the electron vorticity, $\vec{\omega} = \nabla \times \mathbf{v}$, is derived. We find that in addition to the conventional stretching term and baroclinic generation of vorticity (e.g., see [15]), other sources of vorticity are the generation of electron vortices due to the recombination term and decay of vortices due to the momentum relaxation. To simplify our analysis, the diffusion term in the modeling of pressure tensor is neglected. This assumption is valid for high Reynolds numbers and away from the boundaries. For regions close to nonconductive boundaries a diffusion term is needed in the right hand side of the vorticity transport equation to provide a means for the diffusion of the electron vorticity, created at the boundary, into the conductive region. This can be achieved through electron-electron interaction and non-diagonal term in the pressure tensor (viscosity). The rate of vorticity generation at the boundary is set by the boundary conditions. Note that since the electric field is curl free, it does not explicitly appear in the vorticity equation. This is one of the main advantages of this equation. To obtain a complete set of equations of electron transport in semiconductors one needs to supplement the vorticity equation (17) or (19) by an equation for electron dilatation, $\nabla \cdot \mathbf{v}$. This is the topic of a future publication. A scale analysis of the electron vorticity equation is performed and the relative order of magnitude of each source of vorticity is found.

In order to observe electron vortices experimentally, electron transit time in the device should be of the same order or smaller order as the electron momentum relaxation time. Our analysis predict the conditions for the observation of electron vortices in high field transport in submicron devices.

REFERENCES

 P.A. Markowich. The Stationary Semiconductor Device Equations. Springer-Verlag, Vienna and New York, 1986.

- [2] P.A. Markowich, C.A. Ringhofer, and C. Schmeiser. Semiconductor Equations. Springer-Verlag, Vienna, 1990.
- [3] S. Selberherr. Analysis and Simulation of Semiconductor Devices. Springer-Verlag, New York, 1984.
- [4] J.W. Jerome. Analysis of Charge Transport: A Mathematical Study of Semiconductor Devices. Springer-Verlag, New York, 1996.
- [5] C. Jacobini and P. Lugli. The Monte Carlo Method for Semiconductor Device Simulation. Springer-Verlag, New York, 1989.
- [6] K. Hess (ed.). Monte Carlo Device Simulation: Full Band and Beyond. Kluwer Academic Publishers, 1991.
- [7] L. Reggiani (ed.). Hot-Electron transport in Semiconductors. Topics in Applied Physics series, Springer-Verlag, Berlin, 1985.
- [8] M.A. Stettler, M.A. Alam, and M.S. Lundstrom. A critical examination of the assumptions underlying macroscopic transport equations for silicon devices. *IEEE Transactions in Electron Devices*, 40(4):733– 740, 1993.
- [9] A. Shakouri and J.E. Bowers. Heterostructure integrated thermionic coolers. Appl. Phys. Lett., 71(9):1234–1236, 1997.
- [10] K. Blotekjaer. Transport equations for electrons in two-valley semiconductors. *IEEE Transactions in Electron Devices*, 17:38–47, 1970.
- [11] M. Rudan and F. Odeh. Multi-dimensional discretization scheme for the hydrodynamic model of semiconductor equations. *COMPEL*, 5(3):149–183, 1986.
- [12] E.A. Fatemi, J.W. Jerome, and S. Osher. Solution of the hydrodynamic device model using high-order non-oscillatory shock capturing algorithms. *IEEE Transactions on Computer-Aided Design of Inte*grated Circuits and Systems, 10(2):232–244, 1991.
- [13] C.L. Gardner. Numerical simulation of a steadystate electron shock wave in a submicrometer semiconductor device. *IEEE Transactions in Electron Devices*, 38:392–398, 1991.
- [14] M.J.M. de Jong and L.W. Molenkamp. Hydrodynamic electron flow in high-mobility wires. Phys. Rev. B: Condensed Matter, 51(19):13389– 402, 1995.
- [15] G.K. Batchelor. An Introduction to Fluid Mechanics. Cambridge University Press, Cambridge, 1967.
- [16] C. Truesdell. *The Kinematics of Vorticity*. Indiana Univ. Press,, Bloomington, 1954. p. 142.