AN EFFICIENT DISCRETIZATION SCHEME FOR THE ENERGY-CONTINUITY EQUATION IN SEMICONDUCTORS

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Abstract: *In this paper we discuss a discretization method for the energy equation which appears in the hydrodynamic model of the semiconductor equations. We exhibit the robustness of the method through computational results obtained for a realistic quarter micron MOS device.*

A new discretization strategy of the semiconductor equations comprising momentum and energy balance has been proposed in the recent literature [1,2]. The continuous model, for electrons and in steady state, is made of the following equations:

$$\text{div}\mathbf{D} = q\,(\,p - n + N_D^+ - N_A^-\,) \tag{1}$$

$$\text{div}\mathbf{J} = qU \tag{2}$$

$$\mathbf{J} - \frac{\tau_p}{q}\,(\mathbf{J} \cdot \text{grad})\left(\frac{\mathbf{J}}{n}\right) = -q\mu\,n\,\text{grad}(\varphi - k_B T/q) + qD\,\text{grad}\,n \tag{3}$$

$$\text{div}\left[\,-\kappa\text{grad}\,T - \frac{\mathbf{J}}{q}\,(k_B T + w)\right] = \mathbf{E} \cdot \mathbf{J} - n\,\frac{w - w_0}{\tau_w} - wU \tag{4}$$

where $\mathbf{D} = \varepsilon\mathbf{E} = -\varepsilon\text{grad}\varphi$, $\mathbf{J} = -qn\mathbf{v}$, $U = R - G$ are the electric displacement vector, the current density, and the net recombination rate, respectively, while the mobility and the diffusion coefficient are given by $\mu = (q/m)\,\tau_p$, $D = (k_B T/q)\,\mu$, τ_p being the momentum-relaxation time. Finally, $\mathbf{v}$ is the mean velocity, τ_w is the energy-relaxation time, $w = (1/2)\,mv^2 + (3/2)\,k_B T$ is the average energy, and w_0 is the equilibrium average energy.

A discretization technique for the above model has been proposed in [1] as a generalization of the well-known Scharfetter-Gummel (SG) method. The technique has then been refined and applied to two dimensional simulations on a triangular grid [2]. In the procedure presented here, Poisson's and momentum-continuity equations are discretized as in [1] and [2], whereas the energy-continuity equation is treated in a different manner. This is due to the following observations:

- The energy-continuity equation (4) contains the unknown electron temperature T at the LHS in both a "diffusive" term (the one proportional to grad T) and a "drift" term (the one proportional to T). Hence, this equation is structurally similar to the drift-diffusion equation for the current density and, indeed, when the coefficient of the drift term becomes large, it may exhibit the same discretization problems unless the grid is prohibitively refined. This is especially true when solving very small devices, where velocity overshoot is to be expected.

- The forcing term at the RHS of (4) is $\mathbf{E} \cdot \mathbf{J}$, hence special care is necessary to discretize it. This is because, as is well known, the SG scheme does not provide a unique definition of the current density in the interior of the grid elements, which renders the evaluation of the expression $\mathbf{E} \cdot \mathbf{J}$ ambiguous.

In this paper we address the above problems and propose the following solutions. By remembering the expression of the average energy and of the current density, we rewrite Eq. (4) as

$$\text{div}S = -wU - n\,\frac{w - w_0}{\tau_w} + E \cdot J + \text{div}\left(\frac{mJ^2}{2q^2 n^2}\,\frac{J}{q} \right) \tag{5}$$

$$S = -\kappa \text{grad}\,T - \frac{J}{q}\left(\frac{5}{2}\,k_B T \right). \tag{6}$$

Following the SG scheme, Eq. (6) is first projected onto each grid side, say s_{ij}, to yield

$$S_{ij} = -\kappa\,\frac{dT}{dx_{ij}} - \frac{J_{ij}}{q}\left(\frac{5}{2}\,k_B T \right). \tag{7}$$

Eq. (7) is then integrated along the side, assuming that both projections S_{ij} and J_{ij} are constant and replacing κ with a suitable average κ_{ij}. This results in

$$S_{ij} = -\frac{\kappa_{ij}}{s_{ij}}\left[B(\omega_{ij})T_j - B(-\omega_{ij})T_i \right], \tag{8}$$

where B is the Bernoulli function and $\omega_{ij} = -(5/2)k_B\,(J_{ij}/q)\,(s_{ij}/\kappa_{ij})$. Eq. (8) above is sometimes referred to as an "exponential fitting", and is structurally similar to what is found by treating the momentum-continuity equation via the SG method. One may also regard it as a form of "upwinding" scheme used in moderately high Reynold's number flows. The problem of the exponential fitting for the carrier temperature had also been addressed in [2], but a specific form for the thermal conductivity was assumed there. Due to this, the expression of S turned out to be less general and more complicated. Moreover, the integration along the side could be carried out in closed form only after assuming a specific behaviour of the electron concentration along the side.

In the examples presented here, the thermal conductivity κ has been expressed by means of the Wiedmann-Franz law, whose average on the side s_{ij} yields

$$\kappa_{ij} = <\kappa> = (5/2 + c)\,k_B\,D_{ij}<n>. \tag{9}$$

In Eq. (9), D_{ij} is the average of the diffusion coefficient, which is a smooth function as shown in [3,4]. The electron concentration n, on the contrary, can be a rapidly varying function over some elements. Due to this, we have investigated both the dependence of the convergence rate and the sensitivity of the solution on the particular way of evaluating $<n>$. It was found that the way of averaging n plays little role on the solution, whereas the fastest convergence rate was given by either a linear or an exponential average.

As far as the second point above is concerned, the proposed discretization scheme for $E \cdot J$ is based on the simple vector relationship

$$E \cdot J = -\text{div}(q\,J) + q\,\text{div}J \tag{10}$$

which, remembering Eq. (2), leads to the following form of the energy-balance equation

$$\text{div}S = -\text{div}(q\,J) + (qq - w)U - n\,\frac{w - w_0}{\tau_w} + \text{div}\left(\frac{mJ^2}{2q^2 n^2}\,\frac{J}{q} \right). \tag{11}$$

Then, the discretized form of the RHS of Eq. (11) reads

$$\Omega_i \left[(q\varphi_i - w_i) \, U_i - n_i \, \frac{w_i - w_0}{\tau_{wi}} \right] +$$

$$+ \sum_{j \neq i} d_{ij} \left(\, < mJ^2/(2q^2 n^2) >_{ij} - < q\varphi >_{ij} \right) \frac{J_{ij}}{q} \qquad (12)$$

where suffix i refers to the ith node and Ω_i is the area of the ith box. It is worth mentioning that (12) does not involve the problem of computing the current density $\mathbf{J}$ in the neighborhood of the ith node; rather all the physical parameters appearing in (12) are either nodal values of scalar quantities or projections of the current density over the sides emanating from the ith node.

Figs. 1 and 2 show a 3-D plot of the electron concentration and of the normalized electron temperature in a 0.25 μm FET biased with $V_{GS} = 2.5$ V and $V_{DS} = 2.5$ V (different viewpoints have been chosen for the sake of clarity). It is clearly seen how the electron concentration at the drain end of the channel is spread toward the bulk, due to carrier heating and, consequently, to enhanced diffusivity. Consistently, Fig. 2 exhibits a temperature ridge in the vicinity of the metallurgical drain junction and in most of the channel region. As can be seen, near the semiconductor-insulator interface the electron temperature is rather smooth at this refinement level, and is well described up to the drain end of the channel. This confirms that the schemes adopted for the discretization provide satisfactory results, so long as the grid is properly refined. A ripple can be seen, on the other hand, in the deeper portion of the temperature ridge, corresponding to the drain-bulk junction, and is due to coarseness of the grid. Due to the difficulty of *a priori* foreseeing the regions where intense refinement is required, an adaptive scheme based on temperature variation is necessary. Experiments are currently in progress in order to combine the solution of the semiconductor equations with such an adaptive refinement scheme.

References

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Fig. 1

Fig. 2