A Novel Discretization Approach Superior to S-G and SUPG Method

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We often have to solve convection-diffusion equation in many fields, such as aerodynamics, fluid dynamics and microelectronics. If the convection term dominates over the diffusion term, numerical oscillation can result when we use the classical finite element method or central finite difference method. To control the nonphysical oscillation in solution, Scharfetter and Gummel first proposed a discretization method for one dimensional current continuity equation in 1969 (usually, it is referred to as S-G method[1]),then it was extended to two and three dimensional problems(e.g., MINIMOS[2]). However,the S-G discretization method has a loss of accuracy in streamline-normal direction which can be avoided without sacrificing the stability. Usually, the loss of accuracy or numerical dissipation that appears in streamline-normal direction is referred to as a crosswind effect. By adding a linear artificial diffusivity to the Galerkin formula in a weighted residual form, Sharma applied the SUPG (Streamline Upwind /Petrov-Galerkin) method to semiconductor device simulation to eliminate both numerical oscillation and crosswind effects.[3] Unfortunately, the linear artificial diffusivity is not optimal in most cases and is not applicable to some complex current continuity equation other than the drift-diffusion model, e.g., the current continuity equation containing a magnetic field. In this paper, by adding a nonlinear artificial diffusion tensor instead of a linear artificial diffusivity in the streamline direction which satisfies the weighted residual formulation, we derive a novel discretization approach to achieve good stability and accuracy properties simultaneously.

Considering that a nonphysical oscillation usually occurs along with large spurious derivatives of carrier concentration, we can control the wiggles by limiting the derivatives of carrier concentration. For electron current continuity equation: $\nabla\cdot\vec{J}_n=\nabla\cdot(\mu n\vec{E}+D_n\nabla n)=0$, $n|_{\Gamma_1}=n_0$, $\frac{\partial n}{\partial\gamma}\Big|_{\Gamma_2}=0$, $(x,y)\in\Omega$, $\Gamma_1\cup\Gamma_2=\partial\Omega$, we introduce an energy norm $(\int_\Omega \nabla n\cdot\nabla n\, d\Omega)^{\frac{1}{2}}$ and define the corresponding functional:

$$J(n)=\int_\Omega Q\frac{1}{2}\nabla n\cdot D_n\nabla n\, d\Omega \tag{1}$$

where Q is the introduced weighting function to eliminate numerical wiggles. From the minimum condition of J(n) and assuming:

$$\int_\Omega[Q\,\nabla\cdot(\mu n\vec{E})-\nabla Q\cdot D_n\nabla n]\,W\,d\Omega=0 \tag{2}$$

we obtain the generalized Galerkin discretized equation to control wiggles

$$\int_\Omega \nabla W\cdot QD_n\nabla n\, d\Omega=0 \tag{3}$$

where W is the test basis function, Q is derived from equation(2). If we use high order Q function,e.g.

$$Q=\exp\left(\frac{\mu\vec{E}}{D_n}(\vec{r}-\vec{r}_i)\right) \tag{4}$$

equation(3) is equivalent with S-G formula.If we use discontinuous linear Q function in local domain,e.g.,$Q=C_0+C_1x+C_2y$,the present method is similar with SUPG method.

In SUPG method, the weighting residual formula of current continuity equation is

$$\int_{\Omega}\nabla\cdot\vec{J}_n\ (W+\frac{\overline{\overline{D}}_n\vec{v}_n\cdot\nabla W}{|\vec{v}_n|^2})\,d\Omega=\int_{\Omega}qR(W+\frac{\overline{\overline{D}}_n\vec{v}_n\cdot\nabla W}{|\vec{v}_n|^2})d\Omega \tag{5}$$

where $\vec{v}_n$ is the drift velocity vector, $\overline{\overline{D}}_n>0$ is a constant to control numerical oscillation. Comparing(2),(3) with (5),we can construct an optimal artificial diffusivity in the streamline direction which simultaneously precludes the numerical oscillation and crosswind effects,ie,define

$$QW=W+\frac{\overline{\overline{D}}_n\vec{v}_n\cdot\nabla W}{|\vec{v}_n|^2} \tag{6}$$

where Q is given in (4). From (6),we obtain a nonlinear form of $\overline{\overline{D}}_n$ insteading of a constant form:

$$\overline{\overline{D}}_n=\{\exp[\frac{\mu_n\vec{E}}{D_n}\cdot(\vec{r}-\vec{r}_i)]-1\}|\vec{v}_n|^2\ (\vec{v}_n\cdot\nabla\ln W)^{-1} \tag{7}$$

For a n-channel MOS device, where the channel length is 3 μm, the junction depths of drain and source are both 0.8 μm,the substrate doping density is $4X10^{15}$ cm^{-3}, the gate oxide thickness is 80nm,the bias condition is: V_{GS} =0.2V, V_{BS} =0V and V_{DS} =1.5V, we adopt the Gummel algorithm to solve the nonlinear system of Poisson's equation and electron current continuity on a nonuniform rectangular grid.Fig.1 shows the simulated carrier density distributions in the direction normal to the $Si-SiO_2$ interface using the classical S-G method and the present method respectively. In Fig.1, the numerical result using the present discretization method is some different from that using the classical S-G method, the former behaves a higher accuracy than the latter. Also, comparing the channel electric potential distributions using the SUPG approach with that adopting the present discretization method, the numerical result evaluated using the SUPG method has some small wiggles.

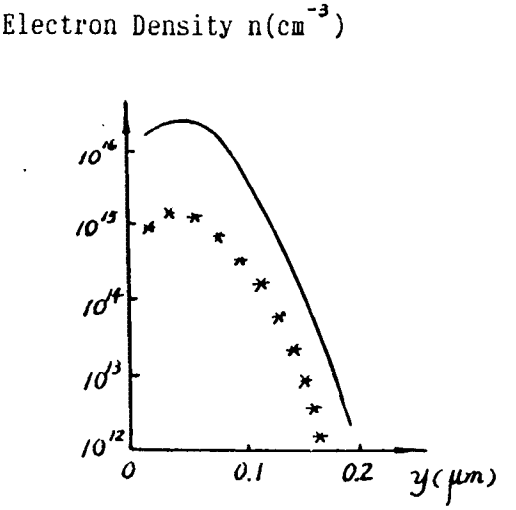

Fig.1 The simulated electron density distributions
* * * The present method —— The classical S-G method

References

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