SEMICONDUCTOR DEVICE SIMULATION: A SPECTRAL METHOD FOR SOLUTION OF THE BOLTZMANN TRANSPORT EQUATION*

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Summary

An efficient numerical method for solving the Boltzmann transport equation in semiconductor device structures has been developed using a basis-function expansion of the distribution function's velocity dependence. This spectral method is ten to one-hundred times faster than the conventional Monte Carlo method for equivalent accuracy.

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Abstract

The description of short length- and time-scale transport phenomena in semiconductor devices necessitates a full dynamical analysis. Under the assumption of semiclassical behavior, the "equation of motion" for an ensemble of charge carriers within an energy-band extremum takes the form of the Boltzmann transport equation (BTE):

$$\frac{\partial f}{\partial t} = -\mathbf{v} \cdot \nabla_{\mathbf{r}} f - \frac{q}{m^*} \mathbf{E} \cdot \nabla_{\mathbf{v}} f + \mathcal{C} f, \tag{1}$$

where $(\mathbf{r}, \mathbf{v})$ are the particle phase-space coordinates, $\mathcal{C}$ is a (possibly nonlinear) integral collision operator, $\mathbf{E} = \mathbf{E}(\mathbf{r}, t)$ is the electric field, and $f = f(\mathbf{r}, \mathbf{v}, t)$ is the distribution function. Here, for sake of simplicity, nondegenerate statistics and a single spherical, parabolic band with effective mass m^* are assumed.

To develop a numerical solution method for BTE (1) a spectral expansion of the distribution function is made,

$$f(\mathbf{r}, \mathbf{v}, t) \approx \sum_{n=1}^{N} \alpha_n(\mathbf{r}, t) \Phi_n(\mathbf{v}), \tag{2}$$

in which the α_n constitute N space- and time-dependent expansion coefficients, and the associated Φ_n are members of a preselected, mathematically complete basis set. Given the Φ_n, equations for the α_n follow through the requirement that BTE (1) be satisfied exactly at N collocation points $\mathbf{v}_k$ $(k = 1, \cdots, N)$, after substitution of expansion (2). The space and time dependence of the expansion coefficients is readily handled using standard finite-difference techniques. It should be mentioned that the earlier work of Rees also employed expansion (2) to develop a numerical solution method [1]. Rees's method, however, is useful only for collision-dominated transport regimes; more importantly, it is impractical for two- and three-dimensional geometries.

Time-independent simulations of device structures for which electrons are injected over a narrow, one-dimensional potential barrier have been carried out. Collisions were modeled with a combination of acoustic and optic phonon scattering processes. Various mathematical basis sets have been used (Fourier, Tchebycheff, Hermite-Gaussian). Maximum accuracy was ensured by collocating at high-order basis-function extrema. The resulting spectral equations were solved by means of Gaussian elimination. All computations were performed on an HP-1000F minicomputer.

A wide range of simulation conditions have been studied, including ballistic and collision-dominated transport regimes. Simulation results have been verified through agreement with physical reasoning, numerical consistency checks, and comparison with other numerical and simple-case analytical solutions.

Spectral solution of the BTE offers great potential in reducing computational effort without sacrificing accuracy. For example, it is estimated that conventional Monte Carlo solution would require an additional factor of ten to one hundred in execution time for equivalent accuracy. The spectral method's numerical efficiency stems from its relatively compact representation of velocity distributions typically found in semiconductor devices.

It is expected that the spectral method can be extended to time-dependent two- and three-dimensional systems in a straightforward manner. In addition, incorporating Poisson's equation should proceed without much difficulty.

References

[1] H. D. Rees, J. Phys. C 6, 262 (1973).