# A Two-Dimensional Device Simulator Coupling the Poisson Equation and Advanced Monte Carlo Transport

S. E. Laux and M. V. Fischetti
IBM T. J. Watson Research Center
Yorktown Heights, NY 10598

A program to model semiconductor devices in two dimensions using a self-consistent coupling of a Monte-Carlo-based transport description and a Poisson solver is described. A complete description of the semiconductor band structure (Si or GaAs) is implemented as part of the transport description. A dedicated graphics program permits the display of either individual particle or ensemble average characteristics. Preliminary results from the simulation of a 0.1 $\mu$m Si n-MOSFET will be described.

# A Two-Dimensional Device Simulator Coupling the Poisson Equation and Advanced Monte Carlo Transport

S. E. Laux and M. V. Fischetti
IBM T. J. Watson Research Center
Yorktown Heights, NY 10598

We describe a program to model semiconductor devices in two dimensions using a self-consistent coupling of a Monte-Carlo-based transport description and a Poisson solver. The DAMOCLES program (Device Analysis using Monte Carlo et Poisson solver) contains a complete description of the semiconductor band structure (Si or GaAs). To date, Monte-Carlo-based device modeling programs have always depended on a simplified (parabolic bands or single parameter non-parabolicity expressions) band description. An analytic form of the band structure is used in valley minima normally populated in equilibrium (X bands in silicon, and Γ, X and L bands in GaAs); a numeric representation of the band structure is only invoked away from equilibrium in order that thermal carriers be simulated as efficiently as possible. A smooth transition between analytic and numeric band models is maintained. Having implemented both analytic and numeric band structure descriptions, we can compare a "full bands" and a "simplified bands" transport model.

The appropriate phonon scattering processes (with anisotropic rates), impact ionization and ionized impurity scattering are included. For all scattering processes except impact ionization, scattering rates are calculated by integrating over the density of final states employing wavevector-dependent matrix elements. This is done to assure the scattering rates are consistent with the "full" band structure. The material and fitting parameters employed in the transport model combine values found in the literature and our own extensive testing; excellent agreement is obtained simultaneously for velocity-field curves, impact ionization coefficients and carrier injection into $SiO_2$ in the case of silicon.

A two-dimensional, finite-difference Poisson solver is used to obtain the self-consistent electric field of the time-evolving electron ensemble. A device geometry (quite flexible within the constraints of rectilinear orientation) and non-uniform mesh structure are readily specified.

DAMOCLES is written in FORTRAN for execution on a IBM 3090 vector processor supporting extended addressing capability. Both CPU and memory utilization are large but consistent with the physical and geometric complexity underlying our calculations.

Finally, a dedicated graphics program has been written to support DAMOCLES. This program permits the display of individual particle characteristics (energy, band index, trajectory) or smoothed ensemble average quantities (electron energy, density, velocity). Animated sequences of these variables can also be displayed. To demonstrate the characteristics of DAMOCLES, we will present preliminary results on the simulation of a 0.1 $\mu$m silicon n-MOSFET.