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Numerical simulation of SiGe HBT's at cryogenic temperatures

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Abstract: This paper describes SCORPIO, a new one-dimensional, drift-diffusion simulator for modeling silicon-germanium heterojunction bipolar transistors (SiGe HBT's) over a wide temperature range (77–400K). SCORPIO will be used to investigate fundamental low-temperature device physics problems and key device design issues. Comparisons of simulation results with experimental measurements are being used to ensure accurate model calibration.

1. THE DEVICE SIMULATOR

SCORPIO (Simulator for Cryogenic Research and SiGe Bipolar Device Optimization) is a newly developed device simulation program for investigating SiGe HBT behavior over a wide temperature range, including (but not limited to) liquid nitrogen temperature (LNT=77K). A simulation tool such as this not only allows for greater understanding of the underlying device physics, but also makes possible the optimization of devices for specific applications. SCORPIO uses a one-dimensional, finite difference, drift-diffusion approximation to model the bipolar device being simulated [1]. The one-dimensional structure used by SCORPIO is shown in Figure 1. Low temperature semiconductor device simulation is a difficult problem because parameters often assumed constant in room temperature (RT=300K) simulators may actually be complex functions of temperature (mobility, for example) [2]. Phenomena unique to low temperature operation, such as carrier freezeout, are typically not accounted for in simulators designed for room temperature use. In addition, the system of equations to be solved at liquid nitrogen temperature is much more ill-conditioned numerically than for room temperature, due to terms having exponential temperature dependencies. For these reasons, typical simulation programs have difficulty converging to a solution at LNT.

SCORPIO has been written in the C++ programming language [3]. Object-oriented programming techniques have been used to simplify the internal representation of data structures such as vectors and matrices. The resulting source code is concise, readable, easy to maintain, and extremely modular. SCORPIO's modularity allows for "plug-in/plug-out" physics, in which modules for simulating various device phenomena may be turned on or off from one simulation to the next. In this way, one can see the differences in using Fermi-Dirac statistics instead of Boltzmann statistics, for example; or compare several different mobility models to see which one agrees most closely with experimental data. This flexibility has been extremely beneficial with respect to calibrating simulation results to measured data because it has allowed numerous models for each parameter to be easily tested in various combinations.

Figure 1. One-dimensional bipolar transistor device model.

1.1. Semiconductor Device Equations

To accurately analyze an arbitrary semiconductor device under various operating conditions, a mathematical model has to be given. The equations which form this model in SCORPIO are commonly called the drift-diffusion equations [4]. SCORPIO attempts to solve Poisson's equation and the electron and hole continuity equations simultaneously for the electrostatic potential (ψ), the electron concentration (n), and the hole concentration (p) as functions of position at a specific temperature. Since these dependent variables (ψ , n , p) are of greatly differing orders of magnitude, the first step towards numerical analysis has to be an appropriate parameter scaling [5], [6]. For the steady-state condition, the scaled (unitless) equations may be written as:

$$\nabla^2 \psi = n - p - N_D^+ + N_A^- \quad (1)$$

$$\nabla \cdot \mathbf{J}_n = R \quad (2)$$

$$\nabla \cdot \mathbf{J}_p = -R \quad (3)$$

$$\mathbf{J}_n = -\mu_n (n \nabla \psi_n - \nabla n) \quad (4)$$

$$\mathbf{J}_p = -\mu_p (p \nabla \psi_p + \nabla p) \quad (5)$$

$$\psi_n = \psi + \chi + \ln(\gamma_n N_c) \quad (6)$$

$$\psi_p = \psi + \chi + E_g - \ln(\gamma_p N_v) \quad (7)$$

The scaled equations are attractive from a computational point of view because they are simpler, and no operations with constants are involved in their evaluation. Note that while (4) and (5) closely resemble the current relations usually used to describe homojunction devices, this particular formulation allows for the bandgap energy (E_g), electron affinity (χ), and densities of states (N_c , N_v) to vary with position. This allows heterostructure device simulation capabilities to be easily implemented [7], and hence permits the simulation of graded-base SiGe HBT's. The influence of Fermi-Dirac statistics has been accounted for through the Fermi correction factors (γ_n , γ_p) [8], allowing a more physically correct simulation, especially at LNT. Advanced parameter models have been implemented in SCORPIO for accurately simulating the effects of carrier freezeout [9], Shockley-Read-Hall and Auger recombination [1], and apparent bandgap narrowing [10]. Doping and temperature dependent majority and minority carrier mobilities are calculated for both electrons and holes [11]. In addition, SCORPIO models the bandgap energy and the conduction and valence band densities of states as functions of germanium mole fraction [12], [13].

For numerical implementation, Eqs. (1)–(7) are discretized on a one-dimensional finite difference mesh. A one-dimensional device model is used instead of a more complex two- or three-dimensional model primarily because, for the bipolar transistor, a one-dimensional structure can successfully simulate much of the device behavior [14]. Additionally, the reduction in complexity of the simulator, and therefore the

required execution time, aids in the use of the program as an interactive design tool. For increased numerical stability, the current density expressions, (4) and (5), are discretized using the Scharfetter–Gummel transformation [15]. Since the equations are nonlinear, an iterative solution technique such as Newton's method must be used.

1.2. The Problem of Convergence at Low Temperature

A difficulty associated with the classical Newton method is the tendency to overestimate the length of the actual correction step for a given iteration. This phenomenon is frequently termed overshoot, and may result in slow convergence (i.e., many iterations are needed to obtain a solution). This problem may be avoided by using a damping parameter to limit the size of each correction step, thus improving convergence [16]. SCORPIO updates this damping parameter after each iteration in an attempt to accelerate convergence.

For every bias condition, Newton's method requires an initial approximation to the solution. If this initial guess fails to sufficiently approximate the actual solution (i.e., if the guess does not lie in the solution's region of attraction) then Newton's method will fail to converge. By default, SCORPIO will first attempt to solve Poisson's equation, assuming zero current flow, to obtain the zero-bias solution. This solution is then passed on to the fully-coupled equation solver. The bias condition is incremented in small steps, using the solution for one bias point as the initial guess for the next bias point. SCORPIO assumes the solver has converged to a solution when the relative error of the Newton update vector becomes suitably small (usually less than 10^{-7}). Convergence difficulty for a given simulation may sometimes be avoided by simply taking smaller bias steps.

Another reason that Newton's method may fail to converge is the loss of numerical precision that may occur due to subtracting nearly equal numbers using finite precision arithmetic. Double precision (8-byte) arithmetic does not provide sufficient accuracy to resolve the solution updates for a given iteration at LNT. The corrupted update vector that results may move the solution approximation for the next iteration outside of the actual solution's region of attraction, and Newton's method will fail to converge. The basic device equations contain both positive and negative exponential functions of temperature. For example, the intrinsic carrier concentration varies over about thirty orders of magnitude from 300K to 77K. As a result, the system of equations being solved becomes more ill-conditioned, and the solution algorithm becomes increasingly sensitive to the effects of precision loss and other sources of numerical error. Thus, obtaining convergence becomes increasingly more difficult with decreasing temperature. To help alleviate this difficulty, critical calculations are performed with extended (16-byte) precision for temperatures below 150K. While the subroutines which use extended-precision arithmetic are slower than those that do not, the extra precision is necessary for converging to accurate low-temperature solutions [17]. At the present time, the lowest temperature for which SCORPIO's zero-bias Poisson solver can successfully converge for an advanced SiGe HBT profile is 20K.

For a 250 node mesh, a RT simulation with SCORPIO typically requires 5–10 Newton iterations per bias step, with up to 100mV bias steps possible for low injection. For high injection, 1mV bias steps may be required. The average execution time is approximately 0.3 seconds per bias step on a Sun SPARC-10 workstation. Convergence at LNT typically requires 10–20 Newton iterations per bias step, with up to 50mV bias steps possible for low injection. For high injection, 1mV bias steps are usually required. The average execution time for LNT simulations is approximately 1.5 seconds per bias step.

2. SIMULATION RESULTS

To demonstrate SCORPIO's usefulness, the realistic doping profile shown in Figure 2 has been simulated at RT and LNT. Note that this profile has been taken from measured SIMS data of an actual state-of-the-art SiGe HBT [18]. This device has a measured current gain of 82, a peak cut-off frequency of 59GHz, and an unloaded ECL gate delay of 28ps at LNT. The arsenic concentration in the emitter has been assumed to be 15% electrically active, and the graded SiGe base has a peak germanium mole fraction of approximately 8%.

Figure 2. Doping profile used in simulator (solid line) compared to actual SIMS data (symbols).

To illustrate the effects of Ge on the device behavior, Figure 3 compares the simulated electrostatic potential in the base of this SiGe HBT to that of a silicon bipolar junction transistor (Si BJT) with identical doping. The smaller bandgap of the SiGe base enhances electron injection into the base. The bandgap grading produced by the germanium profile induces a drift field of about 20kV/cm which enhances minority carrier transport through the base [19].

Figure 3. Simulated electrostatic potential in the base at 300K for a SiGe HBT and a Si BJT.

As a first step towards model calibration, simulated values of the zero-bias pinched base sheet resistance (R_{bi}) were compared to measured data. Reasonable agreement over temperature has been obtained, as shown in Figure 4. R_{bi} increases with cooling due to carrier freezeout in the base. The effects of carrier freezeout can clearly be seen in Figure 5, which shows the simulated hole density in the base at 300K and 77K. Figure 6 compares the simulated versus measured Gummel characteristics in the SiGe HBT at 310K and 84K. The reasonable agreement obtained between the simulated and measured results indicates that the simulator is adequately modeling the dominant temperature dependencies in the device. Improved agreement with measured data is anticipated as further calibrations are made.

Figure 4. Simulated zero-bias pinched base sheet resistance vs. experimental data.

Figure 5. Simulated zero-bias hole concentration in the base at 300K (dotted line) and 77K.

Figure 6. Simulated SiGe HBT I - V characteristics vs. experimental data.

3. SUMMARY

SCORPIO, a simulation tool having robust convergence properties, has been developed for investigating SiGe HBT behavior in the temperature range 77–400K. Strategic use of extended precision arithmetic and careful ordering of mathematical operations help provide rapid convergence at LNT with SCORPIO, even with advanced parameter models and realistic doping profiles. Comparisons of simulation results with experimental measurements are being used to ensure accurate model calibration. SCORPIO is intended to be a useful tool for device optimization and for investigating low-temperature device physics.

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