

**MODELING ELECTRON INJECTION ACROSS SEMICONDUCTOR BARRIERS
IN VLSI DEVICES**

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Electron injection across a barrier is a central feature of bipolar transistor operation. In this talk, we examine electron injection across barriers by four approaches: 1) conventional drift-diffusion simulation, 2) a thermionic emission treatment, 3) Monte Carlo simulation, and 4) by a new, quantum-thermionic emission treatment. The objectives are to establish the essential device physics of the problem, to identify the conditions under which drift-diffusion equations apply, and to discuss what to do when they fail.

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As VLSI devices mature and their dimensions shrink, it is important to re-assess the validity of conventional simulation approaches. Electron injection across a barrier is a central feature of bipolar transistor operation. Despite the fact that drift-diffusion equations are known to fail in such situations, they have been widely, and successfully, used to model devices. But with the continued reduction in device dimensions, and with the advent of sophisticated heterostructure technology, transport across the junction is becoming an important performance-limiting factor. In this talk, we examine electron injection across barriers by using several different simulation approaches and establish the controlling device physics by comparing the results of the various approaches. The objectives are to identify when drift-diffusion equations apply and to describe what to do when they fail. The focus is on AlGaAs/GaAs heterojunctions typical of those employed for heterostructure bipolar transistors (HBTs).

The problem of how to treat electron injection across the emitter-base junction of a bipolar transistor arose in some of the earliest numerical simulation studies when Gokhale pointed out that the use of a field-dependent mobility was unphysical because the electric field cools rather than heats the electrons [1]. He proposed that the gradient of the quasi-Fermi level, rather than the electric field, be used in the field-dependent mobility expression. Since the two approaches produced nearly identical results for conventional silicon BJTs [2], the problem has not been an important one for device engineers. But with the continued down-scaling of device dimensions, mobile charge storage in the emitter-base junction is becoming an important speed-limiting factor in silicon BJTs [3]. More significantly, for AlGaAs/GaAs HBTs, transport across the emitter-base heterojunction is of central importance. For abrupt heterojunctions, drift-diffusion equations have been augmented by a thermionic emission boundary condition [4], but this approach is difficult to justify [5]. Monte Carlo simulation can be applied [6], but electron tunneling must also be treated [7]. Accurate modeling of transport across heterojunctions is a prerequisite to the development of predictive device models for the HBT.

In this paper, we apply standard simulation approaches based on, drift-diffusion transport, thermionic emission, and Monte Carlo techniques, and a new, quantum-thermionic emission technique to the analysis of electron injection across AlGaAs/GaAs

heterojunctions typical of those employed in HBTs. The new technique simulates the collisionless propagation of electron waves across the conduction band profile of a heterojunction. It extends previous treatments [7] because it allows for arbitrary conduction band profiles, reflection of electrons above the potential spike, and can include the self-consistent electrostatic potential. The initial energy band profile is obtained from a conventional drift-diffusion based device model, then the current and carrier densities are computed by assuming that the contacts launch electron waves which propagate without collision throughout the structure. After summing the contributions of incoming electrons distributed over a grid in energy space, the total current and carrier densities are evaluated. For self-consistent computations, Poisson's equation is solved, a new conduction band profile obtained, and the process is repeated until convergence is achieved. The significant assumptions underlying the approach include the neglect of scattering and the use of a simple, parabolic energy band. Neither assumption is expected to compromise the accuracy of the model for use on typical HBT emitter-base junctions.

When a conventional drift-diffusion model is used to evaluate the current-voltage characteristics of an abrupt AlGaAs/GaAs heterojunction, the injected current agrees closely with that obtained by a thermionic emission approach. Curiously, the use of Monte Carlo simulation results in more current because electrons with energy just below the barrier can absorb an optical phonon to surmount the barrier. For typical junctions, however, this effect is relatively small. By contrast, when the quantum treatment is applied to the same problem, the predicted current is more than one order of magnitude greater than that predicted by conventional approaches. We also compare the carrier density profiles predicted by the various approaches because they determine the capacitance and recombination current of the emitter-base junction. Finally, a corresponding study of electron transport in compositionally graded junctions is presented.

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