SELF-CONSISTENT ENSEMBLE PARTICLE MONTE CARLO SIMULATION OF INTRINSIC BISTABILITY IN RESONANT TUNNELING DEVICES

R.E. Salvino* and F.A. Buot
Code 6864, Naval Research Laboratory, Washington, DC 20375
** NRC/NRL Research Associate*

Abstract

We have simulated the intrinsic bistability of a symmetric resonant tunneling device (RTD) by coupling a simple model of the particle dynamics inside the double barrier region of the RTD with ensemble particle Monte Carlo (MC) simulations. The particle motion inside the double barrier region is determined by the tunneling time delays, obtained from an Airy function transmission amplitude calculation. Charge build-up in the well is observed, giving rise to marked bistability and hysteresis in the negative differential resistance (NDR) region of the I-V curve. Plateau-like features of the I-V curve are not seen, although oscillations in the charge density in the NDR are prominent. This strongly suggests that a more accurate treatment of the quantum particle dynamics across the RTD is of paramount importance.

Introduction and Motivation

Self-consistent MC simulations incorporating space and time dependent quantum tunneling are expected to be a very useful tool for simulating the performance and reliability aspects of realistic and multidimensional quantum based devices. As a first step, we have simulated the intrinsic bistability of a symmetric RTD by including a model dynamics for tunneling particles within the framework of traditional MC simulations. This differs from previous work [1] primarily by using dynamics rather than probabilistic insertion into, and extraction from, the quantum heterostructure. Our goal is to fill the need for a dynamical description of transport in quantum structures, in particular, for a dynamical treatment of motion across the RTD to produce the plateau-like behavior in the I-V curve found in more fundamental Wigner distribution function simulations [2].

Computational Method

The double barrier system is sandwiched by bulk semiconductor layers. The total device length is 620 A, each barrier is 30 A wide, the well is 50 A wide, and each spacer layer is 30 A wide. The barrier heights are 0.3 eV. The doping concentration is $10^{18}/cm^3$ with the spacer layers, barriers, and well remaining undoped. The temperature of the system was fixed at 77 K. The Fermi level for the system is determined by inverting the density-chemical potential relation and not by the charge neutrality condition, giving rise to a substantially larger Fermi energy. Each mesh cell is 5 A wide and the doped regions initially

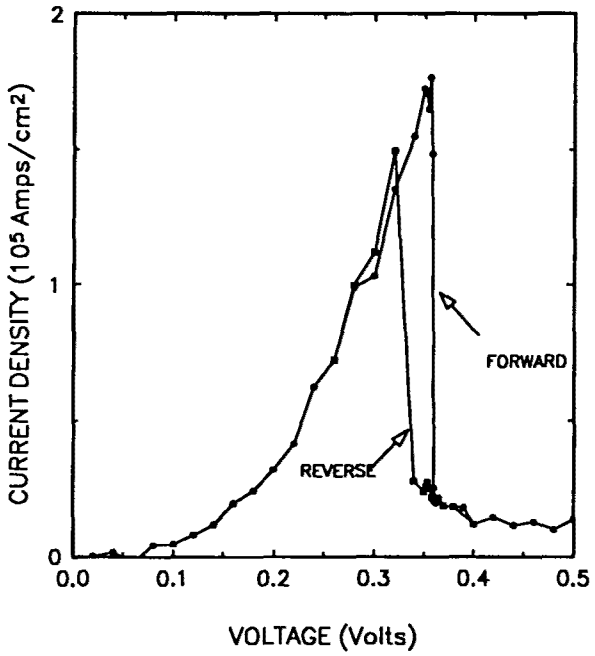

Fig.1. Current–voltage characteristics.

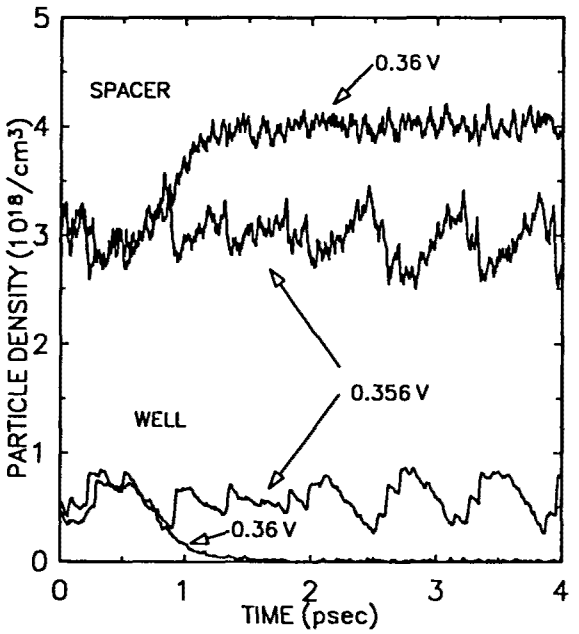

Fig.2. Carrier density in left spacer and well, near peak and low current regions.

contains 20 simulation particles per cell. The initial number of particles in the simulation is 1800. The band structure of the carriers is assumed to be that of GaAs.

Traditional MC simulation describes the dynamics outside the quantum heterostructure. Freeflight times are obtained from scattering rates in the usual way. The scattering mechanisms are acoustic, polar optical, nonequivalent valley, equivalent valley phonons, and ionized impurity scattering. A composite L/X valley constitutes the upper valley. The Poisson fields are calculated self-consistently at every time step, 2 fsec. The standard ohmic contact model at the electrodes uses a Fermi-Dirac distribution for injection purposes. Deviation from the MC algorithm occurs only when particles cross into the quantum heterostructure.

When a particle crosses into the double barrier region of the RTD, it is reset at the barrier edge, using only the time it takes for the particle to reach the barrier edge. A test is then made to determine if the particle tunnels through the structure or not. The transmission coefficient is obtained from a piecewise linear potential approach using the exact solution in terms of Airy functions over the piecewise linear region [3,4]. These coefficients are determined self-consistently at every time step with the Poisson fields. If a particle tunnels, it traverses the barriers with a constant velocity equal to the velocity when it hits the barrier edge; it traverses the well with an adjusted constant velocity corrected by the delay time obtained from the phase of the transmission amplitude [1,5,6]. Reflection is treated as an instantaneous process, and no penetration into the quantum structure is permitted.

Results of the Simulations

Our simulations produce a marked hysteresis loop in the I-V

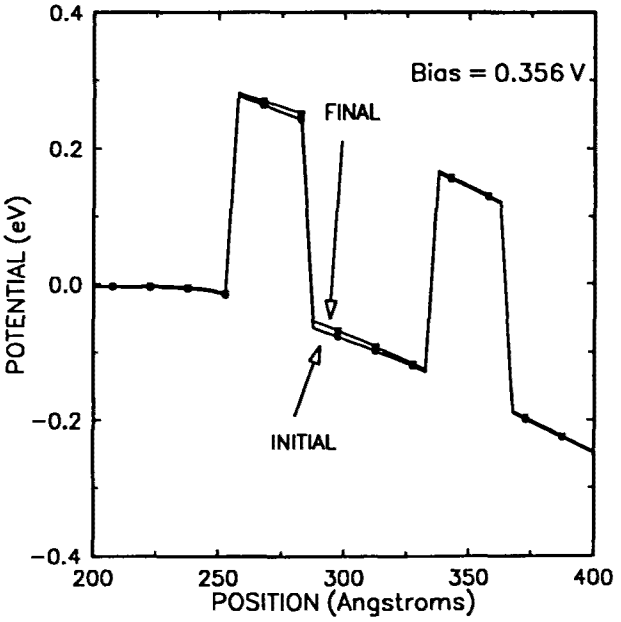

Fig.3. Potential profile at t = 0 and t = 4 psec. Near peak conditions.

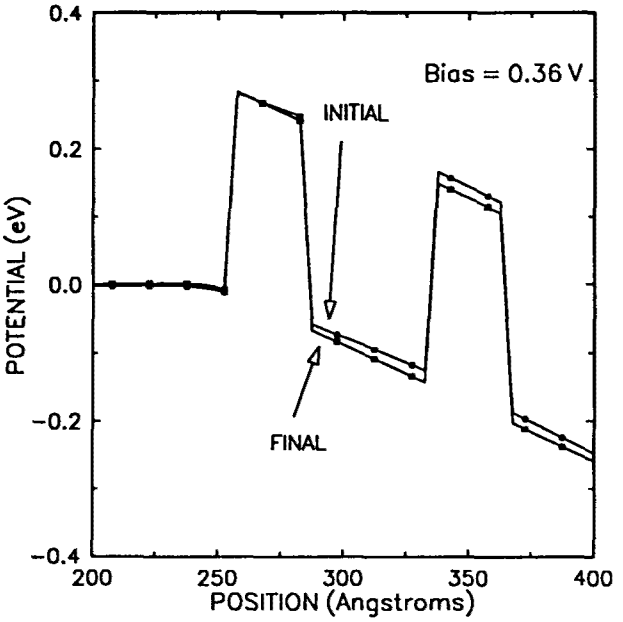

Fig.4. Potential profile at t = 0 and t = 4 psec. Low current conditions

curve (Fig.1). The charge build-up in the well for the forward sweep is clearly in evidence as is the lag in charge build-up for the reverse sweep. However, the plateau regions due to current oscillations are not seen although density oscillations in the in the quantum structure are clearly visible near the unstable region of the I-V curve (Fig.2). These oscillations are initially observed as transients in the particle density in the left spacer region and in the well beginning at a bias around 0.26 V. Near 0.32 V, these oscillations are no longer transient, and remain throughout the duration of the run: the high current region of the I-V curve maintains these density oscillations. At 0.36 V, the well discharges after 1 psec and the density in the well, remaining low, loses its oscillatory character, as does the spacer region (Fig.2). The static nonoscillatory behavior is characteristic of the low current regions of the I-V curve, for both low and high bias. The spacer and well density oscillations are always out of phase.

At 0.356 V, the charge build-up in the well pulls the potential level up relative to the initial configuration (Fig.3). Increasing to 0.358 V shows little change. However, increasing to 0.36 V shows the bias pushes the potential down below the initial potential (Fig.4). The time-averaged behavior for the three cases shows little difference between 0.356 V and 0.358 V potentials and densities, while the 0.36 V shows significant depletion of the density in the double barrier region of the RTD (Fig.5).

The shifting of the peak of the transmission coefficient indicates a different aspect of the "tug of war" between the bias and the charge in the well: the bias pushes the transmission peak toward zero energy, while the charge in the well pulls the transmission peak away from zero energy. For 0.22 V bias (Fig.6), there is not enough charge in the well to compete strongly with the bias. For 0.356 V bias (Fig.6), however, the charge build-up successfully pulls the peak to higher energy. For the catastrophic

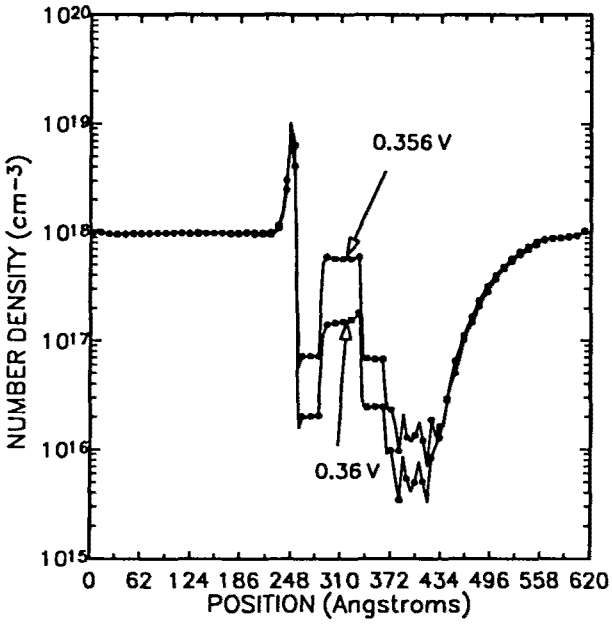

Fig.5. Time averaged density profiles. Near and past peak conditions

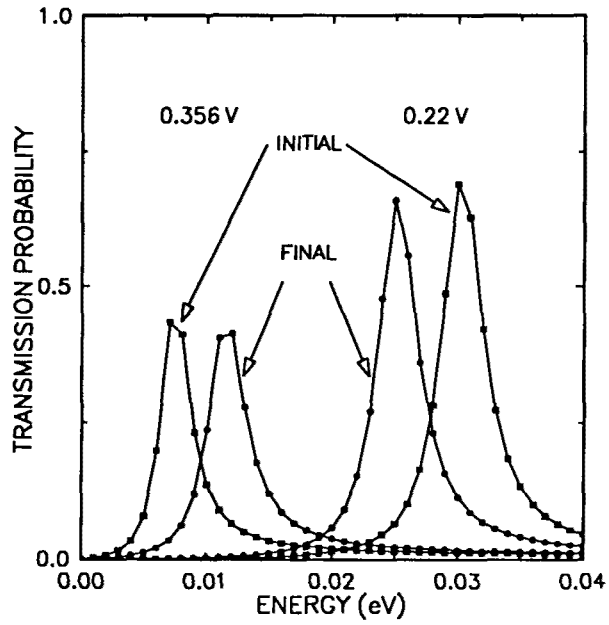

Fig.6. First peak of transmission coefficient. Initial is at t = 0, final is at t = 4 psec

0.36 V bias, the peak disappears in less than 1 psec and never returns. The current stays low until particles can sample the second broad peak in the transmission coefficient. On the reverse sweep, at 0.32 V, the peak reappears in less than 0.5 psec.

Conclusions

We have incorporated a model quantum particle dynamics across the RTD structure in simulating the bistability and hysteresis of a symmetric RTD. We have observed oscillations in the charge density in the quantum well, although these did not appear to translate into current oscillations and the characteristic plateau-like features of the I-V curve. We are working to refine the dynamical treatment in the RTD for this simple transmission coefficient model. We intend to pursue the description of the carrier dynamics of the tunneling particles in MC simulations by two approaches, (1) matching the MC particle trajectory with a Wigner trajectory, and (2) matching the MC distribution function with the Wigner distribution function at appropriately chosen boundaries.

References

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