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Does Circulation in Individual Current States Survive in the Total Current Density?

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Does Circulation in Individual Current States Survive in the Total Current Density?

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Abstract. We describe the two-dimensional simulation of a bent resonant tunneling diode structure which displays vortices in its total current density pattern over a range of applied bias. In contrast, a double gate n-MOSFET is shown where such circulation exists in subband individual states but does not survive in the total current density solution. Both devices are simulated assuming ballistic quantum transport in Si at 300 K.

Keywords: quantum ballistic transport, resonant tunneling diode, double gate FET, circulation, vortex

1. Introduction

The occurrence of vortex excitation in the current flow pattern in a ballistic device for an individual subband state at fixed energy is anticipated and common; for example, see [1-3]. Such circulation will not be properly captured in quantum hydrodynamics device modeling[3]. What is unclear is whether such patterns of circulating current flow can persist in a rigorous total device solution, where a summation over all available occupied energy states and phases present ultimately defines the total current density. Using our program QDAME, which solves the Poisson and Schrödinger equations self-consistently in two dimensions assuming ballistic quantum transport[4-6], we show that this appears possible in a device which limits conduction to a narrow energy window.

2. QDAME

We summarize the physical basis of our program; extensive details are provided in [6]. QDAME is mnemonic for *Q*uantum *D*evice *A*nalysis by *M*odal *E*valuations. The Schrödinger and Poisson equations are solved self-consistently on the same two-dimensional finite element mesh, allowing quite arbitrary device geometries and dopings to be considered. We use a simple six valley, ellipsoidal, parabolic model to approximate the band structure of silicon. The continuous energy spectrum of the quantum system consisting of a device region with open boundary conditions is discretized using the approach of [7]. After first obtaining standing wave solutions in the device domain, we decompose these solutions into their traveling wave constituents, each traveling wave solution associated with injecting at one lead only. This procedure benefits from the use of a modified version of the QTBM[8].

After occupying each traveling state according to a displaced Fermi distribution associated with the injecting lead, the sum over all such occupied states determines the electron density. The electron density is then used to obtain a consistent potential distribution within the device via a solution of the Poisson equation; the procedure iterates until self-consistency is obtained. We ask: while one (or a few) individual current-carrying subband states may display circulation about vortices in their current density solution, is there any possibility that this feature persists in the final device solution, after the summation over all available phases and thermal occupancy factors is performed? We provide an example of a resonant tunneling diode where this appears possible.

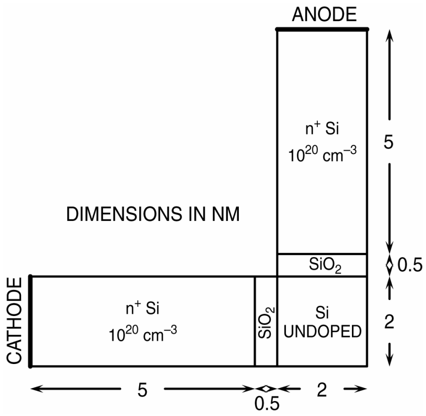

Fig. 1 Bent RTD geometry and doping.

3. Simulation Results

Fig. 1 shows the cross section of a 'bent' resonant tunneling diode (RTD); a straight RTD of similar dimensions is derived from the bent RTD by moving the upper insulator and anode region to the right side of the structure. No variation in the out-of-page direction is assumed. Fig. 2 shows the current-voltage characteristics of both bent and straight RTDs. Note the current axes differ by about a factor of two, consistent with the increased reflection present in traversing a current path that includes a right angle bend. There are two peaks in each case, corresponding to resonant tunneling through the ground state, and the first excited state, respectively, associated with the 2 × 2 nm well region. Judging from these characteristics, the internal behavior of these two devices would seem to be qualitatively the same. For the straight RTD, and for the bent RTD for biases along the lower current peak only, device potentials and densities are completely as expected for an RTD. The current path is either straight through the device (straight RTD) or bends smoothly around the corner (bent RTD). Both devices demonstrate hysteresis, as expected in RTDs.

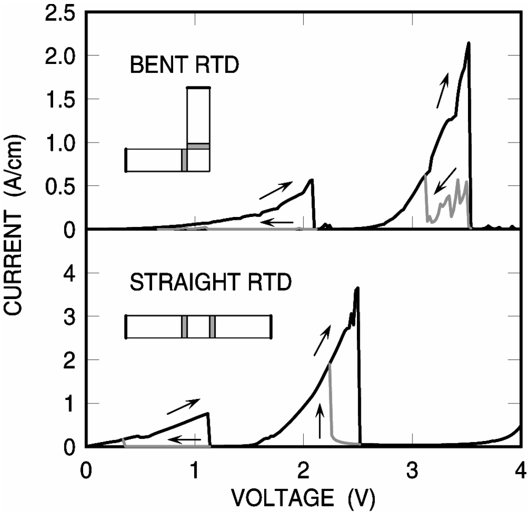

Fig. 2 Current-voltage characteristics of (above) bent and (below) straight RTDs. The inset shows the RTD geometries. The arrows indicate the direction the voltage is incremented to compute the current; hysteresis is found for both RTDs.

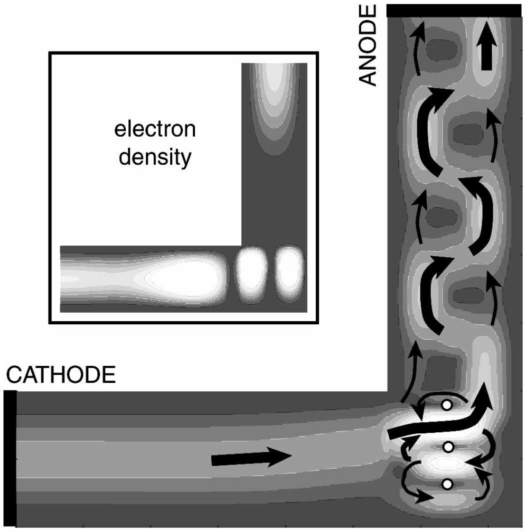

Fig. 3 Contours of the total current density magnitude (light=high, dark=low) of the bent RTD for 3.26 V applied bias (and on the positive voltage increment portion of Fig. 2), with arrows indicating electron movement. Three white dots identify the three vortices in the well region. The inset shows the contours of total electron density, including the 1×2 (vertical × horizontal) nodal structure in the well region.

What is unanticipated is the internal current path for biases along the second current peak in the bent RTD. Fig. 3 shows the very complicated path taken by electrons injected at the cathode for an applied bias of 3.26 V (upper curve of Fig. 2). There are three closed current circulation paths about three vortices, as identified in Fig. 3. In addition, after traveling through the cathode and well regions, electrons leave

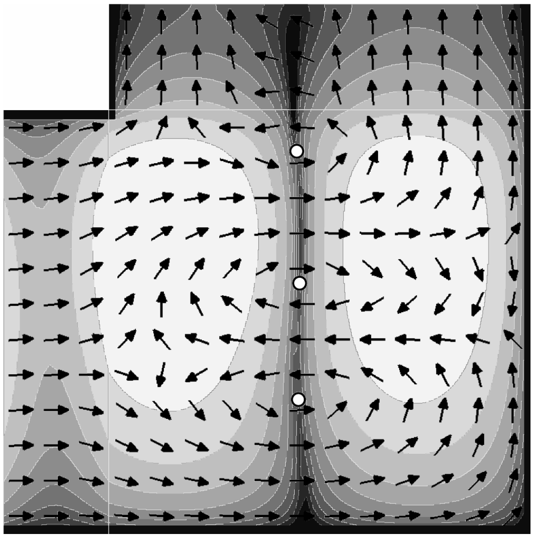

Fig. 4 Contours of electron density , with velocity vectors superimposed. The three vortices are marked with white dots. Only the RTD well and two insulating layers are shown.

the device along a meandering path in the anode. This peculiar current path persists in the total device solution for two reasons. (1) Because of the presence of resonant tunneling, conduction occurs within a very narrow energy window, so the complex current path obtained at the resonant energy also dominates the total conduction in the device. (2) The origin of the meandering path in the anode is explained by considering the classical analog: an electron with forward momentum injected at the cathode will fail to follow the right-angle turn toward the anode exactly, and will bounce back-and-forth off the anode's edges as it continues towards the anode contact. The possibility of being injected precisely into the center of the anode from the well is further diminished by the nodal structure of the electron density as seen in the inset of Fig. 3, since the electron density is very small in the center of the well where it meets the anode. Since the meandering path in the anode is associated with electron charge about two orders of magnitude less than the local doping density, the local electric field does little to attenuate the side-to-side motion of the current carrying electrons.

Note also in Fig. 3 that there are two independent meandering current paths in the anode: the dominant one which turns into the anode beyond the upper vortex, and a weaker flux which turns prior to the upper vortex. These two flows both move from side-to-side in the anode, but out of phase.

As discussed in [9], these 'quantum vortices' are characterized by a velocity solution whose curl is everywhere zero, except possibly at points where the wavefunction (and hence density) is zero. These are precisely the positions where vortices may be found. Fig. 4 shows the well and barrier regions in close-up, indicating that, indeed, the three vortices all occur where the electron density is essentially zero. Again, because of the narrow energy window for conduction, the total electron density in the well displays the behavior anticipated only for an individual subband state. The flow about these vortices must be a closed loop[9]; the electron flow circulating about a vortex does not contribute to the terminal current directly, but rather, only indirectly through the interaction of these electrons with the self-consistent potential and the potential's influence on the determination of current paths. The electron velocity of these closed circuits of current about the three vortices is very nonuniform, as can be seen in Fig. 5. As expected, where the density is small, the velocity must be large to maintain conservation of probability flux.

Least this presence of circulation in the *total* device solution of the bent RTD be misunderstood as commonplace, we show results for a 7.5 nm gate-length double-gate n-MOSFET[4-6] whose solution

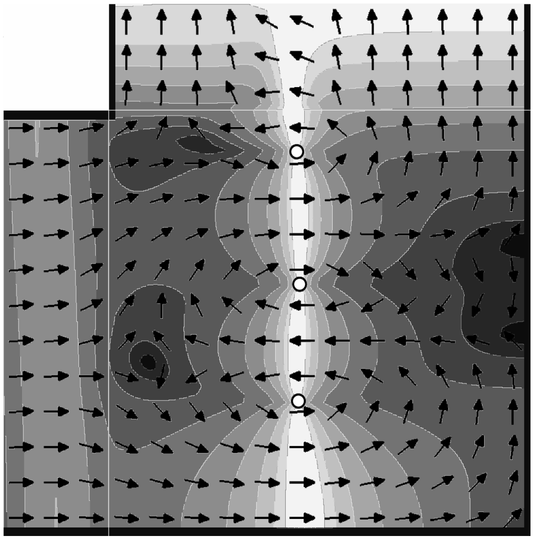

Fig. 5 Same as Fig. 4, except contours of electron velocity magnitude are shown. The velocity is largest along a vertical line through the center of the well.

typifies the usual: the total device current flow is without any sign of circulation (Fig. 6), even though a number of individual one-dimensional subband solutions show circulation. The current associated with one such subband is shown in Fig. 7, where circulation is seen in the source of the FET. Interestingly, for this device structure, individual subband states only demonstrate circulation in the source, or not at all. Thus, these circulating paths seem correlated with the process of electrons moving from a wide extrinsic source into the narrow channel, but not the reverse process in the drain. That is, circulation is associated with reflections inherent in the passage of electrons into the narrow FET channel, and as such, are a sign of 'resistance', in the sense that current flow for a fixed bias is diminished by reflections. In other FET solutions (not shown) which include a roughened Si-SiO_2 interface in the channel[4], circulation is seen in source, channel, or drain[6]. But in every MOSFET case considered to date, the total current flow shows no sign of circulation.

4. Conclusions

In conclusion, we demonstrate that circulation in a ballistic quantum device can, in fact, persist in the total device solution, under appropriate device design and applied bias. Note that this result depends sensitively on the assumption of no scattering in these devices, except for scattering with the device boundaries. The presence of phonon, or even just impurity, scattering in these devices will certainly alter the current flow paths, thereby altering the quantitative, and even qualitative, behaviors reported here. Also, the presence of vortices brings with it the question of their imaginable use; we refer the reader to [10] where their possible application to quantum computing is discussed.

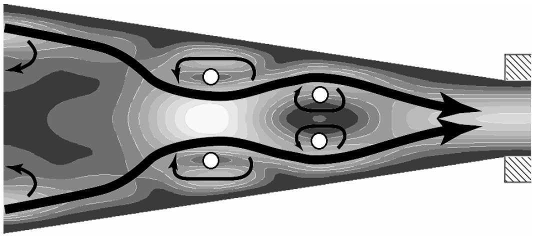

Fig. 7 Contours of the current density magnitude in the source of the tapered FET of Fig. 6, derived from a single one-dimensional subband energy state with total energy 1.1 meV below the source Fermi energy. Electron movement is shown by the arrows, and circulation around four vortices (white dots) is clearly seen.

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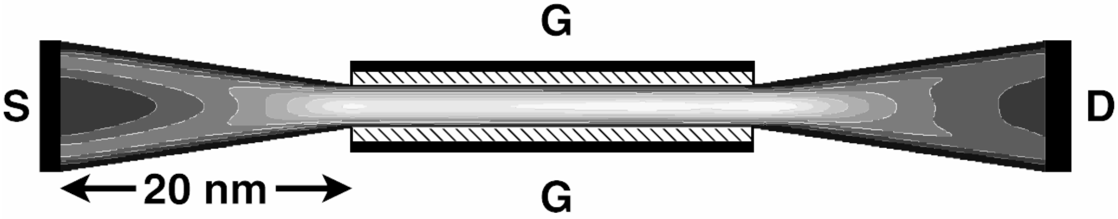

Fig. 6 Contours of the total current density magnitude of a 7.5 nm channel length n-MOSFET. The SiO_2 gate insulation is hatched. Here, V_{GS} = 0.2 V and V_{DS} = 0.4 V. There are no vortices present in the total current density flow.