Implementation of Separable Scattering Mechanisms in Three-Dimensional Quantum Mechanical Simulations of a Silicon Quantum Wire*

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ABSTRACT

We present a numerical scheme through which different phonon scattering processes can be incorporated into the quantum mechanical simulation of semiconductor devices. This method allows the effects of different phonon processes to be seen individually and without resorting to the use of fitting parameters to approximate the correct physics. We derive equations to include acoustic deformation potential scattering and intervalley phonon scattering accounting for both *f*- and *g*- type processes. Using this method we show that we are able to extract the correct mobility for bulk silicon at several different doping densities. The method is then applied to a gated silicon-on-insulator quantum wire device to illustrate the key deviations from the ballistic case that result from the inclusion of these two phonon scattering processes in quantum confined systems.

Keywords: scattering, quantum wire, silicon, simulation, MOSFET.

1 INTRODUCTION

In order to understand the operation of any type of semiconductor device, one must consider the effects of scattering. For many years, Monte Carlo has been the workhorse that has yielded great insight into the operation of a wide variety of semiconductor devices. The Monte Carlo technique handles scattering in a very natural way where quantum mechanical rates are derived from Fermi's Golden Rule and then applied to a distribution of electrons. However, Monte Carlo cannot account for the quantum effects that are seen in future devices. Therefore, other device simulation techniques, such as Green's functions and scattering matrices [1,2], have been proposed which can account for the quantum mechanical effects in these devices in three-dimensions. We have developed a recursive scattering matrix approach to treat ballistic transport in small semiconductor devices [2,3]. In a manner similar to Green's function approaches, but more amenable to the site representation used in these methods, scattering can be computed on a mode basis and then transformed to the site basis. Here, we present results of the first implementation of separable phonon scattering rates in a three-dimensional, fully quantum mechanical, self-consistent device simulation.

2 METHOD

To simulate the devices in this paper, we begin by discretely doping the devices using a method that previously presented in [4]. Once the devices are discretely doped, the dopant atoms are mapped back onto the solution mesh and the Poisson equation is solved for the initial guess at the potential. To include scattering in this approach, as in most semiconductor theory, we treat the scattering as weak. Hence, we can use the Fermi golden rule expression, equivalent to a first-order, non-self-consistent Born approximation, for each scattering process and generate a real space self-energy from it [3]. The scattering rates are then entered into the Hamiltonian for the three-dimensional recursive scattering matrix algorithm [2]. The quantum kernel is started with these scattering rates included and then the density obtained is then fed back into the Poisson equation using the modified Broyden method for updating [5]. This process is continued until a desired level of self-consistency is obtained.

3 RESULTS

We now examine a system—a quantum wire transistor—where the quantum mechanical nature of the scattering matrices is needed to correctly characterize the system. In a system such as this, the phonon scattering should have a more profound effect on the transport, as the reduced area of the wire should give rise to an enhanced overlap integral in the scattering calculations. In the system under consideration, the thickness of the silicon layer is 6.51 nm and the width of the channel is 8.15 nm. The length of the quantum wire that comprises the channel is 9.77 nm in length. Oxide barriers are placed on either side of the channel to simulate the appearance of a hard wall boundary that would be present in an actual experimental system. The source and drain of the device are 18.47 nm wide and 10.32 nm in length. The latter is discretely doped *n*-type with a doping concentration of $1\times10^{20}cm^{-3}$, while the channel is undoped. The quantum wire that forms the

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channel of the device has metal gates on three sides to form a tri-gate type transistor [6]. The gate oxide thickness (SiO_2) on this device is 1 nm. In this simulation, the temperature is taken to be 300 K and the bias across the device is V_{sd} = 0.6 V.

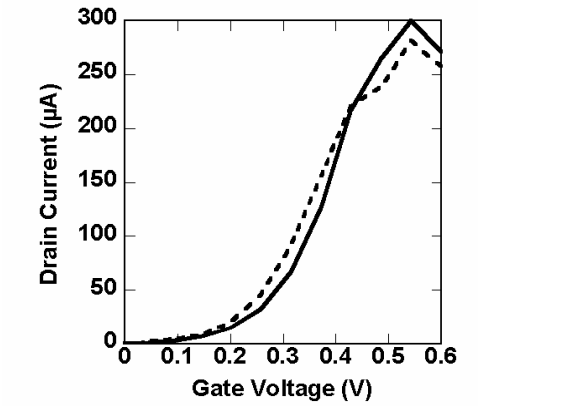

Figure 2: Plot of the I_d-V_g curves for the ballistic (solid) and quasi-ballistic (dashed) for an identical doping distribution with the drain voltage set to be V_d = 0.6 V. Here we see that the inclusion of scattering allows electrons to obtain higher energies that in the ballistic case leading to increased current flow at lower gate biases.

In figure 2, we plot the I_d-V_g curves for the ballistic and quasi-ballistic (only impurity scattering is present) case for an identical doping distribution. The main effect of the phonons on the system is to allow the electrons propagating in the system to scatter to higher subbands, and then back again. This scattering allows the electrons to cross the source-channel barrier at slightly lower gate voltage than in the ballistic case. As the gate voltage increases, the strong effect of the contacts on the charged quantum wire is that quantum interference begins to form in the ballistic case resulting from oscillations seen the conductance both experimentally [7] and theoretically [8,9]. With phonon scattering present, electrons still show these oscillations, but they are damped by scattering. There are more conductance fluctuations of reduced magnitude as the phonon assisted curve has a slight dip near V_g = 0.45 V before it reaches a peak and begins to decline again. However, the ballistic curve increases in typical exponential fashion before the carriers reach levels where they tunnel through the longitudinal states set up in the finite length of the quantum wire.

Oscillations appear not only in the conductance and output current of the quantum wire, but in the density as well. In figure 3 and 4, we plot the electron density at V_g = 0.257 V for the ballistic and quasi-ballistic cases, respectively. One can clearly see the effects of self-consistency in these figures, as the electron density preferentially sits in the potential dips caused by the addition of the discrete donors in the source and drain. In figure 4, we see that the phonon scattering does not lead to a significantly modified electron distribution in the source and the drain of the device (from the ballistic case of fig. 3). However, the electron distribution in the channel of the device is significantly altered. This alteration is caused mainly by the modification of the exchange energy by the influx of scattered electrons in the channel. More electrons in the channel force more of a negative adjustment of the potential by the exchange energy leading to a different charge distribution [8]. While the distribution of the charges is different at each applied gate voltage, we do see a similar pattern of potential oscillations in the channel as the gate voltages are swept.

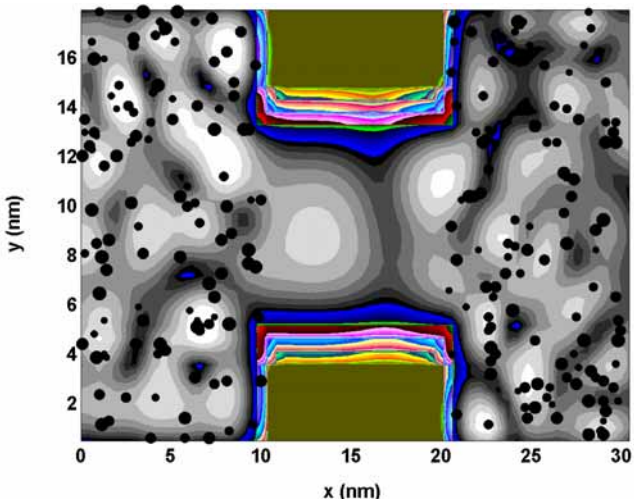

Figure 3: Plot of the ballistic electron density taken in the *xy* plane at a depth of 3 nm in the silicon layer at a gate voltage of V_g = 0.257 V. The black dots correspond to the locations of the dopants with large dots closer to the surface.

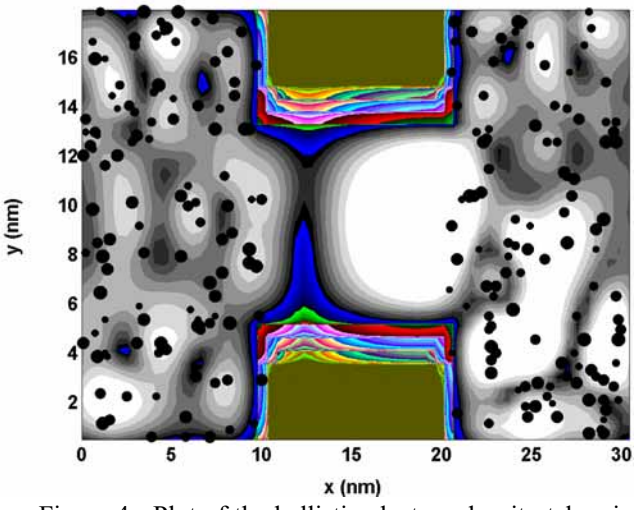

Figure 4: Plot of the ballistic electron density taken in the *xy* plane at a depth of 3 nm in the silicon layer at a gate voltage of V_g = 0.257 V. We find that the scattering into higher subbands creates a channel with higher electron density.

In figure 5, we plot the phonon assisted ballistic to diffusive crossover length for two different drain voltages. In each device, the gate voltage of the channel has been fixed to V_g = 0.5 V to ensure that an inversion layer is present in the channel of the device. We find that at a drain voltage of V_d = 10 mV, the ballistic to diffusive crossover occurs when the channel reaches a length of approximately 1.07 nm (about 2 silicon atoms). This length is much smaller than previously thought which adds additional emphasis to the importance of scattering in these ultra small devices. Further, we find that when the drain voltage is raised to V_d = 100 mV, the ballistic to diffusive crossover occurs at approximately 0.87 nm, or just over 1 silicon atom. This decline in the ballistic crossover length is due to the increased scattering of higher energy carriers.

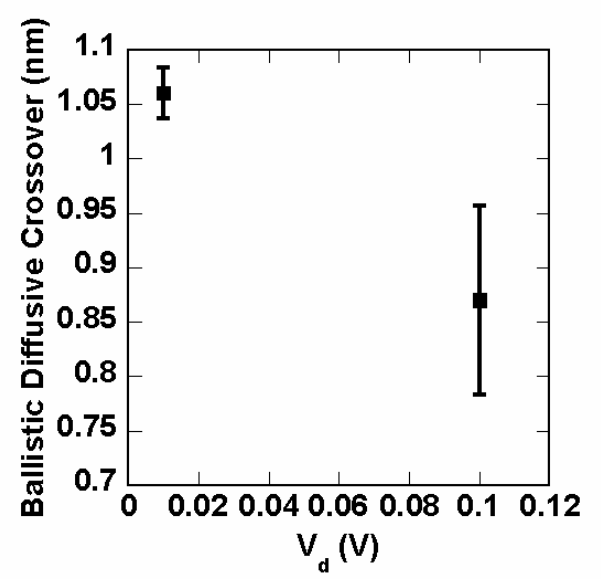

Figure 5: Ballistic to diffusive crossover length for two different drain voltages.

4 CONCLUSIONS

In this paper, we presented a simple physical approach to including separable scattering mechanisms as a self energy in real space. The inclusion of separable phonon scattering mechanisms is crucial in understanding the role that phonon processes play in electrical transport in quantum confined systems. Here, we derived the contributions due to acoustic deformation potential scattering and then proceeded to include this scattering mechanism, as well as intervalley scattering with both *f*- and *g*- type processes, in a simulation of a gated silicon nanowire transistor. We find that the scattering due to phonons causes the electrons to scatter to/from higher subbands than previously available during simple ballistic transport. This modifies the output current by allowing electrons to reach and tunnel through longitudinal states set up in the finite length of the system which causes oscillations in the conductance of the system, and the output current. We also find similar behavior in the electron density, where the influx of electrons over the source-channel barrier into the channel causes the exchange energy to be modified. This modified exchange energy modifies the channel potential causing the electrons to sit in different locations. We also find that the phonon assisted ballistic to diffusive crossover is approximately 1.07 nm at low drain voltages and decreases further at higher drain voltages to 0.87 nm due to enhanced scattering of the higher energy particles.

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