Fully Quantum Mechanical Simulations of Gated Silicon Quantum Wire Structures: Investigating the Effects of Changing Wire Cross-Section on Transport

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Abstract. We present transport simulations of three-dimensional (3D) silicon quantum wires in which electron-phonon scattering is incorporated via local modifications to the potential encountered by the electron waves. Computing resistance as a function of wire length, we find that the effects of dissipation essentially take hold immediately, and are apparent right from the point at which the wire is long enough to act as a true waveguide.

1. Introduction

Recent experiments have shown it possible to fabricate MOS transistors in a Silicon-On-Insulator (SOI) environment with channel widths as small as 2 nm [1-3]. Given the typically small film thickness associated with these devices (≈6 nm), electron transport in such devices should be essentially one dimensional (1D), with electron waves quantized into modes. The semiconductor industry believes that the sizes of what effectively are quantum wires, along with the improved scalability associated with SOI technologies, would be ideal as next generation transistors and interconnects.

With regards to calculating the transport properties of quantum wires, one typically treats the wire as a waveguide and employs a recursive Green’s function or scattering matrix approach. These are straightforwardly provided that the wire is ballistic. However, it is well known that, in a silicon system, transport is not ballistic even for short channel lengths. For realistic calculations applicable to room temperature operation, dissipation must be accounted for in the quantum mechanical simulations. In the silicon quantum wire simulations presented here, this is accomplished by computing the appropriate scattering rates in the waveguide mode basis and then transforming to the site basis, yielding the local modifications to the potential encountered by the electron waves while maintaining current conservation. In this paper, we consider the effect that changing the silicon quantum wire cross-section and length has on the resistance, in order to understand the conditions under which 1D transport and ballisticity are maintained. As we shall show, including electron-phonon scattering produces significant deviations from the ballistic results right down to the length for which the wire can be considered a true waveguide.
2. Calculation

2.1. Description of the Device and the Method

For the device under consideration, the thickness of the silicon layer was 6.51 nm. Oxide barriers were 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 36.93 nm wide and 27.15 nm in length. The source and drain of the device are discretely doped n-type with a doping concentration of $1 \times 10^{20}$ cm$^{-3}$, while the channel is undoped. The quantum wire that forms the channel of the device has metal gates on three sides to form a trigate-type transistor. The gate oxide thickness (SiO$_2$) on this device was 1 nm. Fig. 1 shows a cutaway view of the device, showing source, channel and drain, with dopant positions indicated.

The starting point of the actual quantum mechanical calculation is to map Schrödinger’s equation onto a 3D finite-difference grid. Grouping terms together, one can then derive transfer matrices that allow translation from one 2D slice to the next. Since transfer matrices in themselves are numerically unstable, one does some further manipulation to recast the problem into one that involves an iterative scattering matrix approach [4,5]. In this way, we can obtain the conductance from the transmission coefficients of the quantum wire modes via the Landauer formula. Scattering from dopants and from confining boundaries in this approach is simply included as a local correction to the potential in the Hamiltonian.

To include electron-phonon scattering, 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. This permits us to derive scattering rates expressed in terms of the mode basis of the quantum wire waveguide. At that point, one does a transformation to the site basis, so that the effects of electron-phonon scattering now manifest themselves as local site corrections to the potential. Unlike previous approaches whereby inelastic scattering was included by adding imaginary terms to the Hamiltonian [6], current is conserved using this approach. A fuller description and derivation of this method can be found elsewhere [7]. In the present calculations, the scattering mechanisms that have been included acoustic deformation potential scattering and intervalley scattering with both f and g type processes included.

2.2. Results

For our calculations, the gate voltage was set at $V_g = 0.6$ V, the source-drain bias was $V_{sd} = 0.01$ V. The doping profile was the same in each of the three cases we examined. Fig.1 shows the computed resistance for a device with a channel width of 6.5 nm. At a temperature of 100 K, the electron-phonon scattering is largely suppressed, and in this case resistance quickly rises as a function of channel length and then essentially saturates at $L_{ch} \sim 2$ nm. However, at $T = 300$ K, the resistance continues to rise in a more or less linear fashion. This result is consistent with earlier simulations, done at higher biases, which saw an apparent ballistic to diffusive crossover at $L_{ch} \sim 2$ nm. Note here that the resistance is actually lower for the $T = 300$ K case for very short channel lengths. In this particular case, conditions are such that the electron-phonon scattering is able to excite electrons over the effective barrier created by the channel, thus reducing the resistance, another effect noted earlier.

To understand what is special about $L_{ch} \sim 2$ nm, we also performed a calculation for the ideal, ballistic case. This is shown in the inset. Here, a perfect wire is used without any scattering at all from phonons or impurities, but with simple thermal broadening included using Fermi functions with $T = 300$ K. As is evident, $L_{ch} \sim 2$ nm is the approximate length for which the resistance saturates in the ballistic case. Beyond this length, the wire acts as an ideal quantum point contact (QPC) for which the transmission is quantized and proportional to the number of propagating modes in the wire. The effects of this quantization are evident even with the thermal broadening. However, at shorter lengths, evanescent wire modes that have not decayed can contribute, destroying the conductance quantization and decreasing the resistance.
Fig. 1: Left panel: cutaway overview of the SOI MOSFET device, showing dopant atoms in the source and drain. The interior shading indicates the electron density. For clarity, a relatively long channel length was used to generate this picture. Right panel: resistance vs. $L_{ch}$ for a device with channel width $w_{ch}=6.5$ nm at the indicated temperatures. Inset: result of a calculation for a perfect, ballistic wire without scattering.

Fig. 2: Left panel: resistance vs. $L_{ch}$ for a device with $w_{ch}=4.3$ nm at the indicated temperatures. Right panel: As above, but for $w_{ch}=9.7$ nm

Fig. 2 shows results for a narrower ($w_{ch}=4.3$ nm) and a wider ($w_{ch}=9.7$ nm) channel. As in the first example, the $T=100$ K and $T=300$ K curves here appear to deviate in their behaviour at $L_{ch}$~ 2 nm, indicating that once again that the effects of electron-phonon scattering start to dominate at that length. Both $T=300$ K curves show a kink at $L_{ch}$~ 5 nm (this is also apparent in $w_{ch}=6.5$ nm case, but is less pronounced). We believe this effect is mainly due to the local impurity configuration at the ends of the channel happening to allow for a comparatively enhanced transmission in this particular case. Since we are dealing with discrete dopants that yield local potential fluctuations that can either reflect or draw in electron waves, one should not expect smooth curves without some sort of averaging being done. While the $w_{ch}=9.7$ nm resistance looks approximately linear at $T=300$ K, the $w_{ch}=4.3$ nm resistance appears to rise with a dependence that is more exponential in nature, as if what was being observed was akin to tunnelling. We note here that, at a width $w_{ch}=4.3$ nm, the wire is narrow enough to be near the point of pinch-off, where no modes are transmitted through the wire.
In Fig. 3, results for the three channel widths are compared directly. Clearly, the resistance in the \( w_{ch} = 43 \) nm case rises at a far more rapid rate at 300 K than for the wider channels. At \( T=100 \) K, the wider channels show the \( L_{ch} \sim 2 \) nm saturation behaviour noted earlier, with a simple resistance offset separating the curves. This is consistent with our discussion above about this length coinciding with the establishment of true QPC behavior. Interestingly, the \( w_{ch} = 4.3 \) nm resistance curve for \( T=100 \) K looks somewhat like the \( w_{ch} = 97 \) nm result for 300 K. Clearly, nearer to pinch-off, weaker electron-phonon scattering can have a more pronounced effect on the resistance.

Fig.3: Left panel: direct comparison of the resistance results for the three channel width cases computed at \( T=300 \) K. Right panel: as above, but for \( T=100 \) K.

3. Conclusion
We have performed transport simulations of short 3D silicon quantum wires including electron-phonon scattering, comparing results for different channel widths. At room temperature, we find that the resistance deviates from the ballistic prediction, even down to the length at which the wire becomes a true waveguide.

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