Exchange-correlation effects in ballistic and dissipative transport in GAA Si nanowire transistors

A. Martinez, M. Aldegunde, K. Kalna
College of Engineering, Swansea University
Singleton Park, Swansea SA2 8PP, Wales, UK
a.e.martinez@swansea.ac.uk

J.R.Barker
School of Engineering
University of Glasgow
Glasgow, UK

Abstract—**The impact of exchange and correlation (XC) in the current voltage characteristic of a gate-all-around Si nanowire transistor has been thoroughly investigated in the context of ballistic and dissipative transport. The electron transport is described using the Non Equilibrium Green Function formalism (NEGF). The XC potential is evaluated in the local density approximation. Transfer characteristics for devices with cross-section of 2.2x2.2 nm^2 and 3.6x3.6 nm^2 have been calculated. The calculation shows that the impact of the XC is larger for the small cross-section, producing an enhancement in the on current of close to 50%. This enhancement is gate bias dependent and has a maximum of a few hundred millivolts after the threshold voltage. The impact of the XC in the on current is comparable to the impact of scattering for the small cross-section but it is smaller at the larger cross section.**

Keywords- Silicon Nanowire field effect transistors, Non Equillibrium Green Function formalism, Effective mass approximation, Exchange and Correlation.

I. INTRODUCTION

Many-body effects (MBE), such as dynamic image charge [1, 2] and exchange-correlation [3], affect electron energy levels in the channel of a nanotransistor, as large surface/volume ratios and high electron densities are achieved inside the device. Recent work [1] shows that image charge MBE shifts the top of the barrier down by a 100mV in a 3x3 nm^2 nanotransistor and produces a substantial enhancement in the on-current. The impact of exchange and correlation (XC) on inversion layers [4-5] and on the current-voltage characteristics for 2D device architectures [6] such as double gate, have been investigated in the context of ballistic or semi-classical transport. Furthermore, looking ahead to more predictive device simulations, the quantitative assessment of these effects will become of paramount importance. Nanowire transistors and other 3D architectures have become increasing relevant for the semiconductor industry, as FinFet devices have already been integrated into microprocessor technology by INTEL corporation.

In this work we investigated the impact of the exchange correlation in the I_D-V_G characteristics as a function of the nanowire cross section using a Non Equilibrium Green Function (NEGF) formalism [7, 8, 9]. We have compared ballistics with dissipative simulations. All the phonon mechanisms usually considered in Si Monte Carlo simulations are included [10].

II. PHYSICAL MODELS

The Non Equilibrium Green Function formalism has been used to describe the carrier transport. We used a mode space representation as only few modes are involved in the transport, due to the small cross-section of the wires considered in this work. The Hamiltonian is written in the effective mass approximation [11] but we used confined mass extracted from tight binding calculations. In this paper we considered silicon bulk phonons, which included acoustic and optical. The scattering models and parameters are described elsewhere [12, 13]. The phonon scattering model considered here has been compared with other similar single band model, as well as with full band models. Figure 1 shows the phonon limited mobility as a function of the cross-section and gate bias calculated using the phonon model of this work [14] and of other authors [15, 16, 17]. Note that the results with the full band model [15] are quite striking considering that in ref. Luisier they used full confined phonon dispersion and a more sophisticated model for electron-phonon. The reason is twofold: first at low bias the renormalized (i.e. confinement mass) effective mass seems to be a reasonable approximation and secondly even if the density of states (DOS) of confined phonon is spread, the maximum values of the DOS are concentrated around the bulk phonons used here.

Electron-electron interaction lowers the electron energy by creating a hole (or defect of electrons) around a moving electron. This effect is due to mutual electron repulsion and is well known in strong interacting systems such as metals with high free electron density. The local density approximation (LDA) is one of the most successful and simple approximation used to consider this phenomenon. In this work we have used an improvement of the LDA model due to Hedin and Lundqvist [3]. As this extra interaction energy is beyond the Hartree approximation it is usually called exchange-correlation (XC) energy.

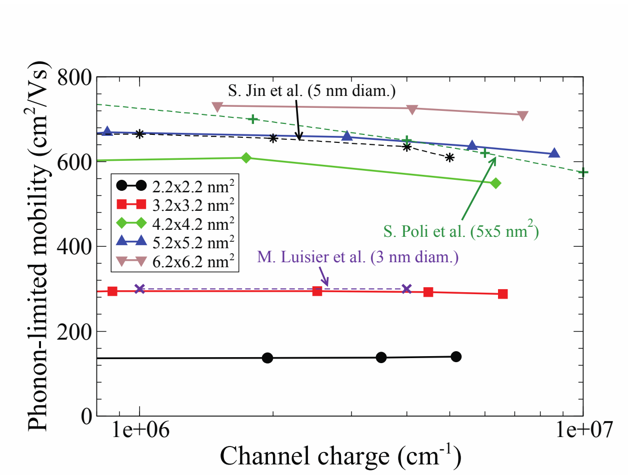

Figure 1. Phonon Limited mobility as a function of the inversion charge. Calculations from references S. Jin [13], S. Poli [16] and M. Luisier [15] are presented for comparison.

III. SIMULATIONS AND DISSCUSIONS

Gate-all-around (GAA) nanowire transistors with 2.2x2.2 nm^2 and 3.6x3.6 nm^2 cross section have been studied. Ballistic and dissipative (phonon scattering) simulations have been carried out. The nanowires have 14 nm S/D and 10 nm channel length and a 0.8 nm SiO_2 thickness. The channel is considered un-doped and the S/D has *n*-type doping concentration of 10^{20} cm^{-3}. The drain bias is set to 100mV.

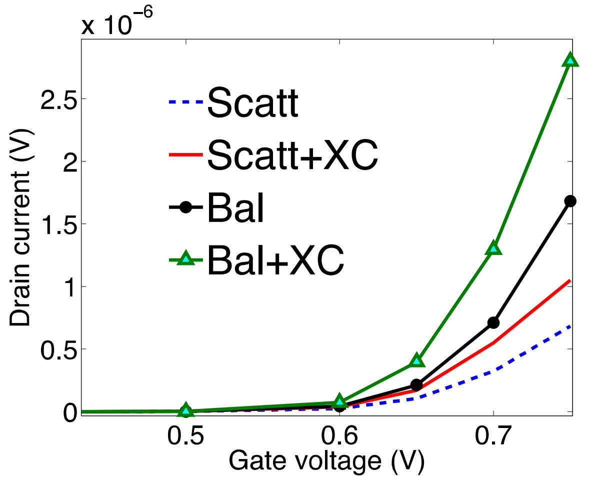

Figure 2. I_D-V_G characteristic for the 2.2x2.2 nm^2 cross-section device with/without X-C and with/without phonon scattering.

Fig. 2 shows the I_D-V_G for the ballistic and dissipative simulations with/without XC for the 2.2x2.2 nm^2 device. Around Vg=0.65 V scattering reduced the on current 50 % as compared with the ballistic one. On the other hand, at the same bias the XC effects improved the ballistic and scattering current by 46 % and 38% respectively. This made the impact of Scattering and XC in the on current similar for this cross section.

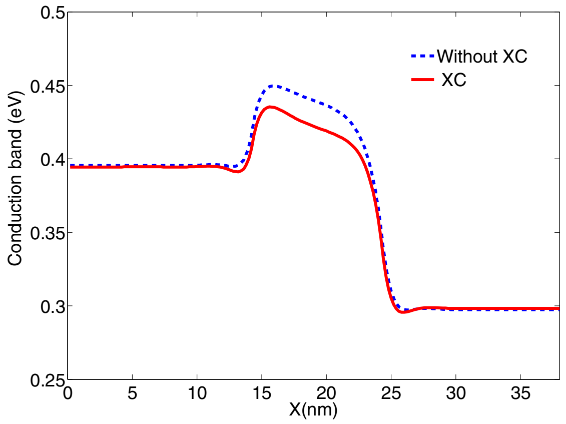

Figure 3. The conduction band profile at Vg=0.7 V for the 2.2x2.2nm^2 cross section device.

The XC potential lowers the source-to-drain barrier resulting in a large drain current as shown in Fig. 3 (conduction band profile for the 2.2x2.2 nm^2 device at V_G=0.7 V). The XC potential has a negligible impact in the sub-threshold region, as the electron concentration in the channel is low.

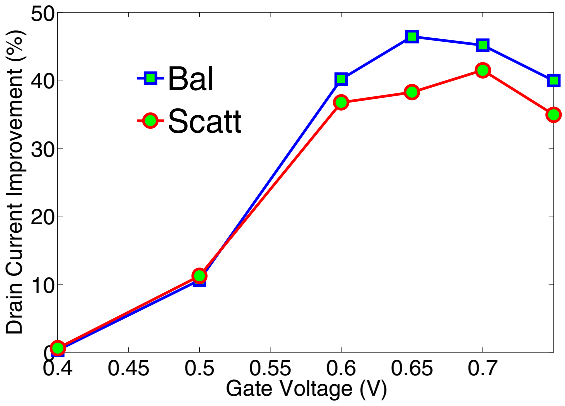

Figure 4. The drain current improvement due to XC for the 2.2x2.2 nm^2 cross-section device with/without phonon scattering

Fig. 4 shows the drain current increases as a function of the gate bias. The shape of the curve is the result of an interplay between source-to-drain tunneling, which tends to minimize the impact of the XC and the electron density in the channel tends to maximize the effect XC. The XC potential increases the on-current current by 40% of its value. The improvement in the drain current is small in the sub-threshold region due to the lower electron density in the channel (under 10%). The current enhancement for the device with scattering is relatively low (35%) when compared to the ballistic device.

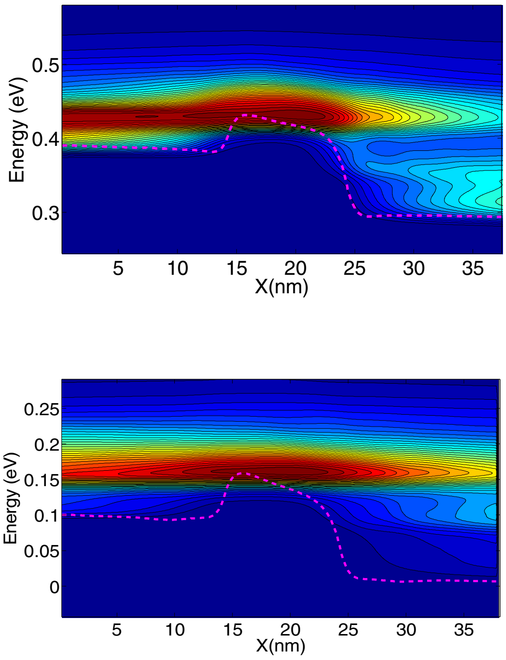

Figure 5. The current spectra along the nanowire cross section at Vg=0.7V. Upper(lower) panel correspond to the small (large) cross-section device.

The spectrum of the current for a 2.2x2.2nm^2 (3.6x3.6 nm^2) device with XC and phonon scattering is shown in fig. 4 (fig.5). There is a large effective electron-phonon coupling for the small cross section device, as compared with the large one. This results in a large spread in the current and the quick relaxation of the electrons at the drain in fig.4 as compared to fig. 5. As a consequence of this, the population of the electrons, which contributed to the current, inverts the population at the drain end as compared to the channel in the small cross-section device. There is significant tunneling in both cases as the channel length is 10 nm but the electrons in the large cross section devices have lower effective masses and therefore larger tunneling probability.

Fig. 6 shows the I_D-V_G for the ballistic and dissipative simulations with/without XC for the 3.6x3.6 nm2 device. The corresponding current enhancement is shown in fig. 7. The effects of the XC in the I_D-V_G are qualitatively similar to the case of the small cross-section device but the effect is lower (30%) partially because the tunneling is stronger. In this device the transversal wave function is broader (less confinement) as compared with the small cross section, inducing a small concentration at the middle of the channel as compared to the small cross section device. The transport in these devices is mainly through the middle of the channel as we are in the inversion volume regime.

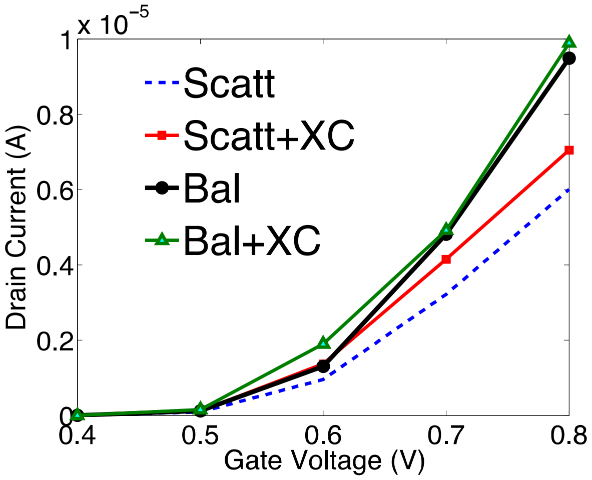

Figure 6. I_D-V_G characteristics for the 3.6x3.6 nm^2 cross-section device with/without X-C and with/without phonon scattering.

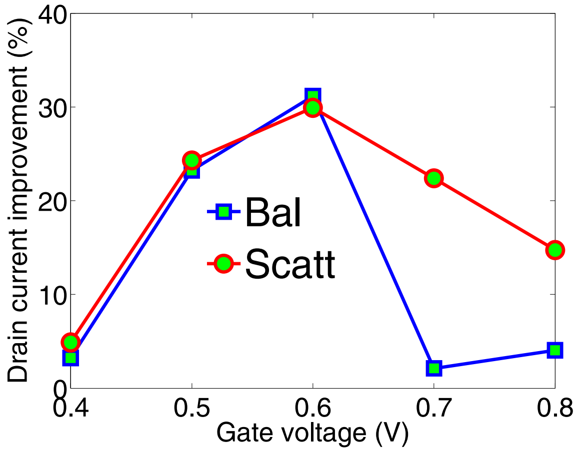

Figure 7. The drain current improvement due to XC for the 3.6x23.6 nm^2 cross-section device with/without phonon scattering

IV. CONCLUSIONS

We carried out 3D non-equilibrium green function ballistic and dissipative simulations for two different cross section (2.2x2.2 nm^2, 3.6x3.6nm^2) gate-all-around Si nanowire transistors. We have evaluated the improvement of the current due to the inclusion of the exchange-correlation potential. The impact on the drain current is strongly dependent on the gate bias. In the sub-threshold region the current enhancement is under 10%, and above the threshold it has a maximum of 50% for the small cross section device. The maximum improvement of the current is 30 % for the large cross section devices. Following the arguments given in this paper, it is implied that the impact of the exchange-correlation will decrease as the nanowire cross-section decreases at least in the volume inversion regime. For the small nanowire cross section the impact of the XC in the on current is of the same magnitude as the impact of the scattering but in the large cross section the effect of XC is smaller. Following the suggestion of Prof. M. V. Fischetti, we believe that an investigation of the XC using a Generalized gradient approximation will be of future value.

ACKNOWLEDGMENT

A. Martinez has been supported by his EPSRC Career Acceleration Fellowship, EP/I004084/1.

REFERENCES

[1] C. Li, M. Becond, M. Lannoo, “GW investigation of interface-induced correlation effects on transport properties in realistic nanoscale structures”, Phys RevB **80**, 195318, 2009.

[2] Y. M. Niquet, “Electronic structure of semiconductor nanowires”, Phys. Rev. B 73, 165319, 2006

[3] L. Hedin and B. I. Lundqvist, “Explicit local exchange-correlation potentials” J. Phys. C: Solid St. Phys. **4**, 2064-83 1971.

[4] D. Vasileska et al, IEEE Trans. Electron Dev **44**, 584-1587 (1997)

[5] H. Iwata, etal, IEEE Trans. Electron Dev **52**, 1596-1602 (2005).

[6] Matthias Sabathil, PhD thesis, unpublished, Munich technical University (2004).

[7] L. V. Keldysh JETP, 47, 1515-1527 (1964)

[8] R. Lake and S. Datta, Non-equilibrium Green function method applied to double-barrier resonant-tunneling diode”, Phys. Rev. B, 45, 6670, 1992.

[9] A. Svizhenko et al., J. Appl. Phys. **91** (4), 2343-2354 (2002).

[10] C. Jacoboni and L. Reggiani, “The Monte Carlo method for the solution of charge transport in semiconductors with applications to covalent materials”, Rev. Mod. Phys. 55, 645–705 (1983)

[11] A. Martinez et al IEEE Trans. Electron. Dev 54(9) 2213-2222 (2007).

[12] S. Jin, M. V. Fischetti, and T.-w. Tang, J. Appl. Phys. 102,083715 (2007).

[13] Jin, Y. J. Park, and H. S. Min, J. Appl. Phys. 99, 123719 (2006)

[14] M. Aldegunde, A. Martinez and A. Asenov, J. Appl. Phys. **110**, 094518 (2011).

[15] M. Luisier, Applied Physics Letters 98, 032111 (2011).

[16] S. Poli and M. Pala, “Channel-Length Dependence of Low-Field Mobility in Silicon-Nanowire FETs,” IEEE Electron Dev. Lett. 30, pp. 1212–1214, Nov. 2009