Impact of oxide thickness on the performance of a GaAs NWFET

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Abstract. Nanowire field effect transistors (NWFETs) are being considered as a replacement for planar MOSFETs at the end of the ITRS. In this work, the change in the relative position of the valleys due to the oxide thickness is investigated, and the subsequent effect this has on the drain current in each valley. An NWFET of cross-section $2.2 \times 2.2 \text{ nm}^2$ and channel length 6 nm has been considered. The strong confinement at this scale can cause the low mass $\Gamma$-valley to become raised in energy, such that it is higher than the heavy mass L and X-valleys. This results in very low current in the device. It was found that increasing the oxide from 0.2 nm to 0.8 nm caused the $\Gamma$-valley to lower in energy, resulting in a higher current. Both ballistic and dissipative transport are considered. This was achieved through the use of the non-equilibrium Green’s function (NEGF) formalism. The mode space approach in the effective mass approximation was deployed, and the conduction band masses were extracted from tight binding simulations. Scattering was found to cause a 65%, 44% and 36% in the current for a 0.2 nm, 0.8 nm and 1.6 nm oxide thickness respectively.

1. Introduction
Nanowire field effect transistors are of interest due to their strong electrostatic control, and are being investigated as an option for the end of the International Technology Roadmap for Semiconductors (ITRS) [1]. Recent advances have led to the investigation of sub-10 nm gate lengths. In this work, we consider gate-all-around NWFETs of cross-section $2.2 \times 2.2 \text{ nm}^2$ and of channel length 6 nm (see figure 1 (a)). The simulated NWFET is n-channel and has a [100] GaAs core. The source and drain are 15 nm long, and are doped at $10^{20} \text{ cm}^{-3}$. The channel is undoped.

III-V nanowires such as GaAs are relevant because of their high electron mobility in comparison to Si. In bulk, the order of valleys in increasing energy are $\Gamma$, L and X (figure 1 (b)). In previous work on $2.2 \times 2.2 \text{ nm}^2$ cross-section gate-all-around NWFETs with a 0.8 nm oxide and 0.2 nm penetration of the wavefunction into the oxide, we found that the $\Gamma$-valley becomes raised in energy, such that it is higher than the L and X-valleys [2]. This is due to the strong confinement and the relatively low mass of the $\Gamma$-valley in comparison to the heavier mass L and X-valleys. In this work, we investigate the effect of increasing the thickness of the oxide and the penetration of the wavefunction into the oxide. We consider a 0.2 nm, 0.8 nm and 1.6 nm oxide thickness, with full penetration of the wavefunction into the oxide.

The Non-equilibrium Green’s function (NEGF) approach is a powerful quantum transport formalism, which has been widely used to simulate nanoscale devices where quantum effects are in existence [3, 4]. In this work, we use the NEGF formalism within the effective mass
Figure 1. (a) A gate-all-around NWFET with a $2.2 \times 2.2$ nm$^2$ cross-section. (b) Bandstructure for bulk GaAs.

approximation (EMA). The effective masses have been extracted from tight binding simulations [5]. Phonon scattering has been introduced through the use of the self-consistent Born approximation.

2. Theory
The NEGF approach describes the modelled system by using the one-particle electronic Green’s functions, $G$, and the self-energies, $\Sigma$. The retarded Green’s function is calculated using

$$G^r(E) = [E_1 - H - \Sigma^r(E)]^{-1} \quad (1)$$

where $H$ is the Hamiltonian of the system. The lesser-than, $G^<$, and the greater-than, $G^>$, Green’s functions are given by

$$G^<(E) = G^r(E)\Sigma^<(E)G^a(E) \quad (2)$$

The advanced Green function, $G^a$, is the complex conjugate of the retarded Green’s function, $G^r$. The retarded self-energy, $\Sigma^r$, is given by

$$\Sigma^r(E) = \frac{1}{2}(\Sigma^<(E) - \Sigma^>(E)) \quad (3)$$

where $\Sigma^<$ and $\Sigma^>$ are the lesser-than and greater-than self-energy respectively.

3. Results
The effect of increasing the oxide thickness is investigated by considering firstly the penetration of the wavefunction for the different oxide thicknesses; the subsequent effect this has on the relative position of the valleys is then investigated. The $I_D-V_G$ characteristics for every simulated NWFET, at both low and high drain bias are included, demonstrating the effect of the oxide thickness on the drain current. Finally, the $I_D-V_G$ characteristics for each valley at low drain bias are included, showing how the current in each valley changes with differing oxide thickness.

The effect of the increasing oxide penetration on the transverse potential energy profile can be observed in figure 2. For the 0.2 nm oxide thickness in figure 2 (a), the potential energy linearly increases as it penetrates the oxide. For the other two cases (b) 0.8 nm thickness and (c) 1.6 nm thickness, the potential energy levels off, after it’s penetrated 0.2 nm into the oxide. The potential energy profile shifts upwards as the oxide penetration increases. The penetration of the wavefunction increases as the oxide penetration increases.

Figure 3 shows the energy-resolved current spectra for the (a) 0.2 nm, (b) 0.8 nm and (c) 1.6 nm oxide thickness. For the 0.2 nm oxide, the $\Gamma$-valley is raised in energy, such that it’s
Figure 2. Transverse potential energy profile and Γ-valley wavefunction for (a) 0.2 nm, (b) 0.8 nm and (c) 1.6 nm oxide thickness.

above the L and X-valley. This is due to the low mass of the Γ-valley in comparison to the heavier L and X-valleys. As the oxide thickness increases, the Γ-valley lowers in energy, such that it is below the L and X-valleys. For the 0.2 nm, 0.8 nm and 1.6 nm oxide thickness, the Γ-valley is 0.65 eV, 0.33 eV and 0.28 eV higher than the potential (denoted by the magenta line) respectively. The subsequent effect this has in the current can be seen in figure 4 (a) and (b), which show the I_D-V_G characteristics at low and high drain bias respectively. As the oxide thickness increases, the drain current increases.

Figure 3. Energy-resolved current spectra for (a) 0.2 nm, (b) 0.8 nm and (c) 1.6 nm oxide thickness (the magenta dotted line is the potential energy profile).

Figure 4. I_D-V_G characteristics at (a) low drain bias, V_D = 1 mV, and (b) high drain bias, V_D = 0.6 V.

Figure 5 breaks down the I_D-V_G characteristics for each valley at low drain bias for the (a) 0.2 nm, (b) 0.8 nm and (c) 1.6 nm oxide thickness. As the oxide thickness increases, the relative
amount of current for the L and X-valleys remains similar, but the relative amount of current in the Γ-valley increases dramatically. For the 0.2 nm oxide thickness, the heavy mass L-valley has the greatest current. However, for the 0.8 nm and 1.6 nm oxide thickness the low mass Γ-valley has the greatest current.

Figure 5. $I_D$-$V_G$ characteristics per valley at low drain bias for (a) 0.2 nm, (b) 0.8 nm and (c) 1.6 nm oxide thickness.

The increase in oxide thickness also effects the reduction in the drain current due to scattering. As the oxide thickness increases, the effect of scattering is reduced. Scattering causes a 65%, 44% and 36% reduction in the on-current for the 0.2 nm, 0.8 nm and 1.6 nm oxide thickness respectively.

4. Conclusions
In previous work on a gate-all-around $2.2 \times 2.2$ nm$^2$ cross-section NWFET, it was found that the strong confinement caused the low mass Γ-valley to become raised in energy such that it was higher than the heavier L and X-valleys. In this paper, the effect of increasing the thickness of the oxide was investigated. Three different oxide thicknesses were considered: 0.2 nm, 0.8 nm and 1.6 nm. It was found that for the 0.2 nm oxide thickness the Γ-valley was above the L and X-valleys, but as the penetration of the wavefunction increased to 0.8 nm the Γ-valley was then below the L and X-valleys. For the 1.6 nm oxide thickness, the Γ-valley was lowered slightly further. For the 0.2 nm, 0.8 nm and 1.6 nm oxides the Γ-valley was 0.65 eV, 0.33 eV and 0.28 eV higher than the potential respectively.

This had a subsequent effect on the current, with the drain current increasing as the oxide increases. This result can be understood by studying the $I_D$-$V_G$ characteristics for each valley. As the oxide thickness increases, the drain current in the L and X-valley changes very little. But as the penetration into the oxide increases from 0.2 nm to 0.8 nm the drain current in the Γ-valley increases by the order $10^4$. The increase in the oxide thickness also reduces the impact of scattering on the drain current. For the 0.2 nm, 0.8 nm and 1.6 nm oxide penetration, there was a 65%, 44% and 36% reduction in the on-current respectively.

References
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