Quantum Transport Studies of InAs Based Nanowire Devices

by

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Graduate Department of Electrical and Computer Engineering
University of Toronto

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Abstract

Experiments and analysis reported in this thesis advance the understanding of quantum transport in nanowire transistors. Indium Arsenide nanowires grown by molecular beam epitaxy were incorporated into numerous back-gated field effect transistors and electronic measurements confirm electron transport is occurring in a regime where ballistic transmission and quantum confinement effects are significant. Quantum interference phenomena are investigated through electrostatic manipulation of interface charge configurations and interference quenching is demonstrated in a nanowire device. Elimination of interference distortions reveal perfect quantization of the conductance and provide direct insight into the one-dimensional quantum-electronic bandstructure which displays strong divergence from cylindrical hard-wall confinement. Numerical simulations investigating morphological
variations demonstrate a strong influence on electronic sub-band structure, prompting characterization of the cross-sectional morphology via focused ion beam micro-sampling and transmission electron microscopy. Adoption of hard-wall confinement potentials consistent with the characterized morphology indicates significant electrostatic influence of interface charges on the sub-band structure.
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Introduction, Background and Overview

1.1 Introduction

Since its advent nearly 70 years ago, the transistor has assumed a central position in our technological landscape and forms the fundamental building block for nearly all electronic devices. As the field continues to progress, conventional three-dimensional transistor technologies are reaching their fundamental limits and researchers are turning to novel structures and materials to ensure continued advancement in performance. In particular, semiconducting nanowires have emerged as promising candidates for future transistor technologies. These quasi one-dimensional structures offer distinct advantages in terms of integration density and their one-dimensional geometry open the doors to gate-all-around architectures which can significantly boost electrostatic gate control resulting in faster switching speeds and reduced power
consumption$^{1-4}$. Furthermore, the strong coupling to their environment makes nanowire structures ideal for sensing applications. Strong sensitivity to single charges has already been established$^5$ and functionalization of their surface has enabled detection of various chemical and biological species$^6-8$.

As the sophistication of growth techniques continue to develop, nanowire structures are being created with near perfect crystalline quality enabling carriers to propagate through these channels ballistically (i.e with little or no scattering). Furthermore, control of nanowire diameters to dimensions smaller than the electronic wavelength result in quantum confinement of carriers and associated quantization of the electronic energy structure.

1.2 Background

Quantum Confinement in Nanostructures

In semiconductor transport the band structure is commonly modeled via the effective mass approximation (EMA). In this model, the effects of the periodic potential within the crystal lattice are accounted for by the so-called effective mass of the electron ($m^*$), and the electrons are treated as free particles with mass equal to the effective mass. Within the constructs of this model, the Schrödinger equation relating to electrons in the conduction band takes the following form:

$$\left[ E_c + \frac{-\hbar^2}{2m^*} \nabla^2 + U(r) \right] \psi(r) = E \psi(r) \quad (1.1)$$
Where \( \psi(\mathbf{r}) \) is the wave function at position vector \( \mathbf{r} \), \( E \) is the total energy, \( U(\mathbf{r}) \) is the potential at position \( \mathbf{r} \), \( m^* \) is the effective mass, as discussed above, and \( E_c \) is the energy of conduction band minimum.

The solution to this differential equation takes on the form of a plane wave \( \psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \) and the energies are given by \( E = E_c + \frac{\hbar^2|\mathbf{k}|^2}{2m^*} \) where \( \mathbf{k} \) is the wave vector with components \( k_x, k_y \) and \( k_z \) which satisfy the equation \( k_i = n(2\pi/L_i) \) where \( n \) is an integer and \( L_i \) is the sample dimension in the \( i = x, y \) or \( z \) direction. Thus for macroscopic samples where \( L_x, L_y \) and \( L_z \) are all large, the spectrum of allowed energy states appear continuous. Conversely, when carriers are confined in one, two or three spatial directions such as in the case of quantum wells, wires and dots respectively, the discrete nature of the energy states are increasingly pronounced and can no longer be treated as a continuum in the confinement direction.

![Density of states for bulk (3D) and confined (2D, 1D and 0D) structures](image)

*Figure 1.1: Density of states for bulk (3D) and confined (2D, 1D and 0D) structures*
Dispersion Relation in One-Dimension

In the case of cylindrical nanowires the effective-mass form of the Schrödinger equation can be most readily solved in cylindrical co-ordinates where \( z \) is the longitudinal co-ordinate whose axis coincides with the longitudinal axis of the wire, \( r \) is the radial co-ordinate and \( \phi \) is the azimuthal co-ordinate. For a nanowire with radius \( R \) and length \( L \gg R \) the system can be modeled as having infinite length. Applying hard-wall boundary conditions whereby \( U(r, \phi, z) = 0 \) for all positions where \( r \) is less than the nanowire’s radius of \( R \) and \( U(r, \phi, z) \to \infty \) for all positions where \( r \geq R \) gives the following solution to the effective mass form of Schrödinger’s equation:

\[
\psi_{n,l,k_2}(r, \phi, z) = \left( \sqrt{\pi R J_{l+1}}(\alpha_{n,l}R) \right)^{-1} J_{l} \left( \frac{\alpha_{n,l}R}{R} \right) e^{\pm il\phi} e^{-ik_2z}
\]

(1.2)

Where \( J_l \) is the \( l^{th} \) order cylindrical Bessel function of the first kind and \( \alpha_{n,l} \) is the \( n^{th} \) root of \( J_l \). It is important to note that this wave function can be expressed as the product of two independent wave functions \( \psi_{n,l,k_2}(r, \phi, z) = \varphi_{n,l}(r, \phi) \Phi_{k_2}(z) \) where \( \Phi_{k_2}(z) = e^{-ik_2z} \) and \( \varphi_{n,l}(r, \phi) = C_{n,l} J_{l} \left( \frac{\alpha_{n,l}R}{R} \right) e^{\pm il\phi} \) where \( C_{n,l} \) is a constant of normalization with value \( C_{n,l} = \left( \sqrt{\pi R J_{l+1}}(\alpha_{n,l}R) \right)^{-1} \). Thus, the longitudinal wave function \( \Phi_{k_2}(z) \) has the form of a regular plane wave. The axial wavefunctions \( \varphi_{n,l}(r, \phi) \) are plotted in Figure 1.2a for the first 6 subbands.

According to standard quantum theory

\[
E_{n,l}(K) = \left\langle \psi_{n,l,k_2}(r, \phi, z) | H | \psi_{n,l,k_2}(r, \phi, z) \right\rangle
= \left\langle \varphi_{n,l}(r, \phi) \Phi_{k_2}(z) | H | \varphi_{n,l}(r, \phi) \Phi_{k_2}(z) \right\rangle
\]

(1.3)
\[ = E_{n,l}^* + \mathcal{E}_{n,l}(k_z) \]

Where \( \mathcal{E}_{n,l}(k_z) = \hbar^2 k_z^2 / (2m^*) \) is the regular plane-wave dispersion relation for the \( n, l \) sub-band and \( E_{n,l}^* = \hbar^2 \kappa_{n,l}^2 / (2m^*) \) is the \( n, l \) sub-band minimum with \( \kappa_{n,l} \) taking on values \( \kappa_{n,l} = \alpha_{n,l}/R \). Thus for a sufficiently small radius wire, each sub-band will be well separated in energy as illustrated in Figure 1.2b.

Figure 1.2: (a) Wavefunction probability density for the first six sub-band modes assuming hardwall cylindrical confinement potential. (b) Dispersion relation for the first three sub-bands\(^{10}\).
Density of States in One-Dimension

In the case of one-dimensional structures, each sub-band has the form of a plane wave. Accordingly the allowed k-states take the form \( k = n2\pi/L \) where \( n \) is any positive or negative integer. From this relationship it can be readily shown that the total number of states \( N(k) = \frac{L}{2\pi}k \times 2 \), where a factor of 2 has been included to account for spin degeneracy. Thus, the density of states with respect to \( k \), \( \frac{dN(k)}{dk} = \frac{L}{\pi} \).

This density can be expressed with respect to the kinetic energy by applying the chain rule \( \frac{dN}{d\epsilon} = 2 \frac{dN}{dk} \frac{dk}{d\epsilon} \), where an additional factor of 2 has been included to account for the positive and negative \( k \) values for a given \( \epsilon \). Since the solutions to the wave equation in the longitudinal direction take the form of a plane wave, the kinetic energy relates to \( k \) via \( \epsilon = \frac{\hbar^2 k^2}{2m^*} \) which gives \( \frac{dk}{d\epsilon} = \frac{m^*}{\hbar^2} = \frac{\sqrt{m^*/2\epsilon}}{\hbar^2} \). Thus \( \frac{dN}{d\epsilon} = \frac{2L}{\pi} \frac{\sqrt{m^*}}{2\hbar^2 \epsilon} = \frac{L}{\hbar \pi} \frac{\sqrt{2m^*}}{\epsilon} \). Finally, dividing by length \( L \) gives the density of states per unit energy per unit length for the \( n, l \)th sub-band as:

\[
g_{n,l}(\epsilon_{n,l}) = D_{n,l} \frac{1}{\hbar \pi} \frac{\sqrt{2m^*}}{\epsilon_{n,l}} \tag{1.4}
\]

Where \( D_{n,l} \) is a degeneracy factor which accounts for the number of sub-bands with identical minima and dispersion relations. The overall density of states can be obtained by summing over all sub-bands yielding:

\[
g(E) = \sum_{n,l} \mathcal{H}(E - E_{n,l}^0) \frac{1}{\hbar \pi} \frac{\sqrt{2m^*}}{E - E_{n,l}^0} \tag{1.5}
\]
Where \( \mathcal{H}(x) \) is the well known Heaviside step function defined by
\[
\mathcal{H}(x) = \begin{cases} 
0, & x < 0 \\
1, & x \geq 0 
\end{cases}
\]

**Landauer Formalism and Ballistic Transport**

The dynamics of ballistic transport through one-dimensional structures was first developed by Landauer\textsuperscript{11,12} and lead to the monumental conclusion, that in the absence of scattering, conductance is precisely quantized in units \( 2e^2/h \) per conducting sub-band.

We begin by considering a 1D channel connected to left and right leads with quasi-Fermi energies \( \mu_1 \) and \( \mu_2 \), respectively. In the case where only a single sub-band is occupied, the current through a two terminal device of length \( L \) can be expressed as the sum of right and left moving currents:

\[
I = \frac{e}{L} \left[ \sum_{k > 0, \sigma} T(k)v(k)f_L(k) - \sum_{k < 0, \sigma} T(k)v(k)f_R(k) \right]
\]

(1.6)

Where \( T(k) \)is the transmission probability for a carrier of wavevector \( k \), \( v(k) \) is the velocity of the carrier and \( f_L(k) \) and \( f_R(k) \) are the distribution functions of the left and right reservoirs respectively. Substituting for carrier velocity \( v(k) = \frac{1}{\hbar} \frac{\delta E}{\delta k} \) and converting sums over wavevectors \( k \) and spin \( \sigma \) to integrals over energy results in the following expression for the current,

\[
I = \frac{2e}{\hbar} \int T(E)(f_L(E) - f_R(E)) \, dE
\]

(1.7)
After noting that \( f_L(E) - f_R(E) \approx (\mu_L - \mu_R) \frac{\partial f}{\partial E} \) for small differences in potential across the structure, the linear conductance can be written as

\[
G = \frac{2e^2}{h} \int T(E)(-\frac{\partial f}{\partial E}) \, dE
\] (1.8)

which can be extended to the case of multiple occupied sub-bands by introducing transmission probabilities \( T_{ij}(E) \) for carriers which have been scattered from sub-band \( i \) to sub-band \( j \)

\[
G = \frac{2e^2}{h} \sum_i \int \left(-\frac{\partial f}{\partial E}\right) \sum_j T_{ij}(E) \, dE
\] (1.9)

In the case of a fully ballistic one-dimensional channel complete transmission occurs (i.e. \( T_{ij} = \delta_{ij} \)) and the conductance is given by

\[
G = \frac{2e^2}{h} \sum_n \frac{1}{1 + e^{\frac{E_n - E_F}{k_B T}}}
\] (1.10)

Which at temperature, T=0 K, simplifies to

\[
G = \frac{2e^2}{h} M
\] (1.11)

where \( M \) is the number of sub-bands or “modes” with cut-off energies below the Fermi level \( E_F \) of the channel. Thus, in fully ballistic wires the conductance is expected to be quantized in units of \( \frac{2e^2}{h} \).
Quantum Point Contacts

The first realization of fully ballistic one-dimensional transport in semiconductors was achieved nearly thirty years ago in structures known as quantum point contacts (QPCs)\textsuperscript{13,14}. In these structures, a high mobility two-dimensional electron gas (2DEG) formed at the interface of a GaAs-AlGaAs heterojunction is shaped into a quasi one-dimensional electron gas (1DEG) through the action of two Schottky contact split-gates which electrostatically define the spatial distribution of electrons. A schematic for a typical QPC structure is depicted in Figure 1.3a.

When the gate electrodes are unbiased the 2DEG exists throughout the entire region between the source and drain contacts, however at negative gate biases the 2DEG is depleted in the region underneath the gate electrodes as well as laterally from the electrode edges forming a one-dimensional channel between the gates. For more negative gate potentials the depletion regions will extend laterally and the effective width of the channel will shrink. As the Fermi-wavelength is comparable to the channel width, the crystal momentum will be well quantized and the gate potential will control the number of sub-bands which can propagate through the constriction. Furthermore, as the length of the one-dimensional channel is far shorter that the mean free path, carriers will traverse the constriction ballistically resulting in a quantization of conductance in units $2e^2/h$ for every propagating mode. This gives rise to a stepwise conductance with respect to gate potential, where each step corresponds to the propagation of carriers through an additional sub-band.
Ballistic Transport in Nanowires

Despite the remarkable success of QPC structures in achieving ideal ballistic one-dimensional transport, the confinement in these structures is defined by depletion regions resulting in confinement potentials which are parabolic in nature. This limits the achievable strength of the confinement in these structures and restricts their usability to ultralow cryogenic temperatures (~1K). On the other hand, the hard-wall confinement potentials inherent in nanowire structures make them attractive systems for realizing one-dimensional transport. Control of nanowire diameters to extremely small scales has enabled observation of one-dimensional behaviour at room temperature\textsuperscript{16}. Furthermore, the ability to grow nanowires from low effective mass materials such as InAs\textsuperscript{17-20} and InSb\textsuperscript{21,22} strongly increases the confinement energies over GaAs which is typically used in QPC structures.

Semiconducting nanowires have garnered much interest in the past 15 years and there have been numerous reports of conductance quantization in various III-V as
well as Ge semiconductor nanowires and metallic carbon nanotubes\textsuperscript{23-34}. Nevertheless, surface charges create inhomogeneities in the channel potential which scatters carriers and leads to interference between carrier wavefunctions. Such effects distort or even wash-out the conductance spectrum from the ideal quantized stepstructure expected in ballistic devices and have been a major barrier to the understanding the transport and energy structure in nanowire devices.

Figure 1.4: Conductance spectra of various quasi-ballistic nanowire structures from reports in the literature. All $G$ vs $V_G$ traces display significant distortions from an ideal step-structure. (a) GaAs/AlAs core-superlattice nanowire\textsuperscript{35} (b) carbon nanotube\textsuperscript{23} (c) InAs nanowire\textsuperscript{36} (d) Ge-Si core-shell nanowire\textsuperscript{25}
1.3 Overview

In this thesis the one-dimensional electronic transport in InAs nanowire transistors is studied in a regime where quantum confinement and ballistic transmission play significant roles.

In Chapter 2 an outline of the relevant procedures for fabricating the nanowire field effect transistors is presented as well as an overview of the measurement apparatus and methodologies.

Chapter 3 explores coherent transport phenomena in the nanowire devices. Weak localization measurements are presented as a means of probing the degree of coherence through the structures and are performed at various temperatures to correlate the loss of coherence with phonon interactions. Furthermore, the role of disorder induced quantum interference in obscuring the one-dimensional band structure is explored, and the significance of surface charge configurations on the overall interference process is illustrated. An example of quenching this interference through electrostatic manipulation of surface state configurations is presented, thereby enabling clear observation of six sub-bands in the conductance spectrum.

In Chapter 4 a numerical model for the G vs $V_G$ relation is developed for a cylindrical nanowire, and compared to experimental findings. Sub-band energies and dispersion relations are calculated by solving the effective mass form of the Schrodinger equation assuming hard-wall confinement potentials. Carrier densities are calculated using Fermi-Dirac integrals, the capacitance is modeled using electrostatic finite element simulations employing the relevant geometry and the gate potential is related to the
Fermi energy through a charge control model. Conductance is then calculated by adopting Landauer formalism for ballistic channels.

Chapter 5 explores the significant role of cross-sectional morphology on the one-dimensional band structure in nanowires. Previous assumptions of cylindrical cross-sections are relaxed, and hexagonal morphologies are adopted. We investigate the effect of deviations in geometry from the regular hexagon and map out the sub-band spectra for a specific class of deviations. After establishing the significance of morphological variations, we characterize the cross-sectional geometry of the interference quenched nanowire by two different techniques. First, the wire is ruptured by joule heating and the cross-section is imaged by angled high resolution scanning electron microscopy. In addition, a focused ion beam microsampling technique is employed to prepare a cross-sectional slice of the nanowire which is then characterized via transmission electron microscopy. The sub-band energy spectrum associated with the observed geometry is calculated and compared with experimental measurements.

In Chapter 6 we explore electrostatic contributions to the confinement potential and illustrate how experimental sub-band spectra could serve as a fingerprint of interface state densities.
Fabrication and Measurement Methodologies

2.1 Fabrication

Electron Beam Lithography

The fabrication of all devices studied in this thesis relied on a specialized nanofabrication technique known as Electron Beam Lithography (EBL)\textsuperscript{37}. This technique enables the precise patterning of structures with critical dimensions as small as a few nanometres\textsuperscript{38}. In the context of this work, the EBL process was employed to create metallic markers for locating wires, source, drain and top gate electrodes, bonding pads as well as the metallic traces which connect the electrodes to the bonding pads.
The first step in the EBL procedure involves coating the substrate in an electron sensitive film known as a “resist”. This process, known as spin coating, involves dispersing a solution of the resist over the sample and then spinning the sample at high angular velocity to create a uniform layer over the sample. The sample is then baked to evaporate the solvent, leaving behind a solid layer of the resist material. The thickness of the resist layer can be tuned by adjusting the spin speed as well as the concentration of the resist solution.

Following the spin coating process, an EBL system selectively exposes the surface of the sample to a highly focused electron beam according to a user defined pattern. Exposure of the resist to an electron beam causes physio-chemical changes to the resist material which alter its solubility. In the case of negative resists, which are exclusively used in this work, exposed regions transition from low to high solubility and can be preferentially dissolved by a developer solution.

The development process leaves windowed regions in the resist where it was exposed to the electron beam. Subsequent deposition of metallic layers adhere to the substrate in these windowed regions however in all other areas the metallic layers affix to the resist. A process known as “liftoff” then removes these resist-affixed layers by dissolving the resist, leaving behind the substrate-affixed layers in the regions defined by the lithography.
Figure 2.1: Schematic of the electron beam lithography process. (a) Resist coating (b) Lithographic patterning via electron-beam (c) Development (d) Deposition of metallic layers (e) Lift-off (f) Final metalized pattern³⁹
Fabrication Methodology

Figure 2.2: (a) Three dimensional representation of Hafnia capped InAs NWFET in the back-gate configuration. (b) Cross-sectional schematic of NWFET. (c) Colourized scanning electron micrograph of NWFET.

Nanowire devices were fabricated on 500μm thick degeneratively doped p⁺ silicon substrates (resistivity 0.002-0.005 Ω-cm) with a 100nm thermally oxidized SiO₂ layer. In addition to providing a structural base, the substrate acts as a functional component of the NWFETs with the degeneratively doped Si layer functioning as the global back gate electrode and the oxide layer as the gate dielectric.

Exposing the nanowires to an electron beam can lead to hydrocarbon contamination which degrades the performance of transistor devices. This is especially true in the case of nanowire transistors where the surface to volume ratio is so large. For this reason, the use of a scanning electron microscope (SEM) was avoided for locating suitable nanowires and an optical microscope was employed in its place. To precisely determine nanowire co-ordinates, a grid of indexed markers spaced 50 μm apart was created on the substrate via standard electron beam lithography techniques.
A solution of suspended InAs nanowires was created by sonicating an ~1mm² section of growth substrate in 1mL of 2-Propanal (IPA). Wires were transferred to the substrate by drop-casting approximately 10μL of the solution via micropipette. The solution was allowed to dry and the substrate was subsequently immersed in a 60°C bath of IPA for 10 minutes followed by a DI water rinse to remove impurities which precipitated from the drying process.

The substrate was then imaged with a Nikon LV100 microscope at the Toronto Nanofabrication Center (TNFC) and suitable nanowire coordinates were identified relative to grid marker locations.

In preparation for lithography, substrates were spin coated with a bi-layer of ebeam resists. First an EL-7 copolymer layer is spun at 4000 RPM followed by a 90 seconds bake at 180°C on a hotplate. Next, a layer of PMMA A3 is deposited in the same manner. The purpose of the bilayer scheme is to aid in the liftoff of thicker metallic patterns. The copolymer resist is more sensitive to the electron beam which results in an undercut in the resist profile. This aids in the liftoff process by reducing the likelihood of bridging connections forming between the metallic layers on the surface of the resist and the windowed pattern regions.

Once the substrate has been coated with the resists, it can be loaded into the EBL system and source/drain contacts with 400nm widths spaced 1μm apart were patterned over selected nanowires. The source and drain patterns connect to larger gauge traces which run to 200μm square bonding pads. Following the lithography, samples were developed in 1:3 solution of IPA and Methyl Isobutyl Ketone (MIBK)
solution for 1 minute followed by a rinse in IPA and then deionized (DI) water. Samples were then dried with Nitrogen gas. Patterns were descummed in a mild oxygen plasma to remove residual resist from the patterned regions. The plasma was generated by a commercial McCarroll cavity operated at 70 Watts of power at 2.45 GHz under 100mbar of oxygen.

To ensure good ohmic contacts to the wires, samples were submerged in a 0.3% by weight Ammonium Polysulfide solution in DI water for 7 minutes. The use of ammonium polysulfide has been shown to promote ohmic contacts to InAs by etching the native oxide and terminating the surface with sulfur atoms, which help to pin the surface of the wires high in the conduction band\textsuperscript{40,41}. Following the passivation, samples were rinsed with DI water dried in N2 gas and then quickly loaded into a Physical Vapour Deposition (PVD) system for metallization. First, 10nm of Ti is deposited by an Electron Gun (E-Gun) source followed by 100nm of Au by a thermal source. The thin Ti layer helps to promote good adhesion to the SiO2 substrate. Lift-off was performed overnight in acetone, and samples were cleaned in NMP stripper to remove any residual resist, followed by Acetone, IPA and DI water rinses.

Samples were then shipped to the National Enterprise for Nanoscience and Nanotechnology (NEST) in Pisa, Italy where approximately 10nm of HfO\textsubscript{2} dielectric was deposited via atomic layer deposition to form a passivating capping layer over the NWFETs.

Returned substrates were then then cleaved into a 5mm x 5mm section and mounted on 28-pin leadless chip carrier (LCC) via indium bonding. The substrate’s bonding
pads are then connected to the pins of the chip carrier via a commercial wedge style wire-bonder (Kulicke and Soffa model 4526) and the chip carrier is loaded into the measurement system.

![Images](image1.png)

Figure 2.3: (a) Optical determination of nanowire co-ordinates relative to pre-patterned grid marker. (b) Optical micrograph of large and small traces connecting to the source and drain electrodes of a NWFET. (c) Optical micrograph of large traces connecting to the 200 micron square bonding pads. (d) Device chip wire bonded to leadless chip carrier\textsuperscript{10}.

2.2 Measurement Setup

Electrical characterization of devices were carried out in a closed cycle Helium cryostat (Advanced Research Systems DE 202) at temperatures ranging from 10-300
Kelvin\(^*\). Temperatures were monitored with a Silicon diode sensor (Lakeshore DT-670) and controlled via resistive heating coils connected to the PID feedback circuitry of a Lakeshore model 330 temperature controller. A custom built copper chip holder was screw mounted to the end of the cryostat’s cold finger, sandwiching an indium foil gasket to ensure good thermal grounding. The copper holder housed a G10 plastic fixture with 24 spring loaded contact pins. The LCC sits on top of the probes and is fixed in place by a copper top plate which presses the LCC contacts against the spring loaded fixture probes to ensure good electrical and thermal contact. The back of the fixture probes are soldered to the ends of a cryogenic ribbon cable which connects to the external atmosphere via a hermetically sealed electrical feedthrough. These connections run to a RF shielded electrical breakout box which employs toggle switches to divert the leads of the device under test (DUT) to the various electrical instruments or to the ground via 1M\(\Omega\) resistors. The grounding resistors were crucial in protecting the devices from electrostatic damage (ESD) when disconnected from electrical instrumentation.

DC gate and source/drain biases were provided by source-measurement unit (SMU) of a commercial semiconductor characterization system (Keithley 4200) which enabled simultaneous sourcing and measuring capabilities. The AC source/drain signal \(V_{ds}\) was provided by the output of a low frequency lock-in amplifier (Stanford Research Systems SR830) operating at a frequency of 210 Hz to avoid potential interference from 60 Hz power line harmonics. The signal passed through a 1/10

\(^*\) The baseline temperature was limited to 15-20K for periods of the project due to issues with the cold head
voltage divider network before being inductively coupled to the DC signal via a signal transformer (Triad Magnetics). The combined signal is routed to the breakout box where it is attenuated once more by a 1/100 voltage divider network before routing to the drain pin of the DUT. Therefore, the total input voltage $v_{DS} = V_{DS} + v_{ds} = V_{SMU}/100 + v_{lock-in}/1000$ (The lock-in output was set to 500 $mV$ for all measurements which after voltage division translates to a small signal of 500 $\mu V$ at the drain electrode of the DUT). The small output current from the source electrode of the DUT is routed to a low-noise current preamplifier (Ithaco Instruments model DL1211) with typical gain settings of $10^{-6}$ A/V. The preamplifier output is routed back to a lock-in where the signal is read.

Magnetic field dependant transport measurements were achieved by lowering the sample end of the cryostat between the poles of an adjustable gap electromagnet (Alpha Scientific model 4600). The electromagnet was powered by an Alpha Scientific model 3002 power supply which was in turn controlled via an Agilent E3631A programmable power supply. Direct measurement of the field strength via a Lakeshore 450 gaussmeter enabled calibration of the programmable power supply and correlating powers could be swept to produce fields with intensities ranging from -0.6 to 0.6 T

The cryostat was evacuated to a pressure of less than $10^3$ mbar via turbomolecular pumping (Balzers TPU 240) for a minimum of 10 hours prior to measurements. This reduced the amount of adsorbed species on the surface of the sample which are known to deleteriously influence the transfer characteristics and mobility of nanowires.
Figure 2.4: (a) Device mounted on cryostat chip holder. (b) External view of the cryostat and electromagnetic system. (c) Circuit schematic for differential conductance measurements. (d) Circuit schematic for breakout box.
Coherent Transport and Quantum Interference

3.1 Introduction

Over the small length scales inherent in nanoscale devices, the true quantum mechanical nature of carriers manifest in a multitude of phenomena which are absent in macroscopic devices. In keeping with this quantum description, carriers are described as wave packets with a complex-valued probability amplitude given by the general form $\psi = Ae^{i\varphi}$, where $\varphi$ is referred to as the phase of the wave packet. Accordingly, when two waves combine the probability amplitude is given by

$$P = |\psi_1 + \psi_2| = |A_1|^2 + |A_2|^2 + 4|A_1 A_2| \cos (\varphi_1 - \varphi_2)$$  \hspace{1cm} (3.1)

Thus the probability is dependent on the phase relationship between the carriers and can vary from a maximum value equal to the sum of the two amplitudes, when the carriers are in phase, and a minimum value equal to the difference of the two
amplitudes, when the carriers are out of phase. This concept of superposition of wavefunctions results in a multitude of quantum interference phenomena\textsuperscript{13,43-45} which usually manifest as oscillations in the conductance. In order for these phenomena to be observed, the phase information of carriers must be preserved which only occurs over a characteristic length, $l_{\varphi}$, known as the phase coherence length which is limited by inelastic scattering events such as electron-electron, and electron-phonon interactions. In macroscopic samples transport occurs over length scales which are much larger than the coherence length and the summation of small coherent sections combine stochastically to average out any interference effects. In nanoscale structures, such as those studied in this thesis, this is not the case and quantum interference effects play a significant role in the transport which we illustrate in the following sections.

### 3.2 Weak Localization

The weak localization effect was first described in the works of Anderson and Gorkov\textsuperscript{46} and served to explain the apparent reduction in conductivity observed in diffusive samples at low temperatures. To understand this effect we consider carriers propagating through a sample which are subject to a multitude of scattering events. The probability of such carriers traversing from point $\mathbf{r}$ to $\mathbf{r}'$ is given by

$$P(\mathbf{r}, \mathbf{r}') = \left| \sum_i A_i \right|^2 = \sum_i |A_i|^2 + \sum_{i \neq j} A_i A_j^*$$  \hspace{1cm} (3.2)
Where $A_i$ is the probability amplitude for trajectory $i$. The $\sum_i |A_i|^2$ term in the above equation corresponds to the classical diffusion probability however the $\sum_{i \neq j} A_i A_j^*$ term corresponds to the contribution from quantum interference. When there are a great number of trajectories which contribute to the sum one can expect that this interference term will average out since the phases will be uncorrelated. This is indeed the case for differing start and end points $\mathbf{r}$ and $\mathbf{r'}$, however, if we consider closed loop trajectories where $\mathbf{r}$ and $\mathbf{r'}$ are coincident this does not hold. Time invariance symmetry guarantees that carriers traversing the same close loop path in the clockwise and anticlockwise direction will be equally as likely. Since carriers will accumulate the same phase in both cases, this results in constructive interference at the starting point and results in doubled probability of backscattered carriers compared to the classical case leading to a reduction in the sample conductance.

![Diagram](image)

Figure 3.1: Schematic of carrier wavefunction propagation from starting point $\mathbf{r}$ to end point $\mathbf{r'}$ along different trajectories (a) different start and end points (b) co-incident start and end points where trajectories form a closed loop path. Propagation in the clockwise and anti clockwise direction are equal.
Suppression of Weak Localization by Magnetic Field

The application of a small perpendicular magnetic field will act to diminish the weak localization correction to the conductance. This follows from the fact that the magnetic field will have an opposite affect on the phase of carriers propagating in the clockwise and counter clockwise trajectories. Accordingly, there will be a relative phase shift between the two trajectories which will reduce the constructive interference at the starting point thereby reducing the probability of coherent backscattering. This translates to an increase in sample conductance with increasing magnetic field.

![Graph](image)

**Figure 3.2:** Magnetoconductance measurement for a bare InAs nanowire at temperatures ranging from 15-75K
In Figure 3.2 the magnetoconductance measurements for a bare InAs nanowire FET is presented and illustrates that the transport is influenced by coherent interference. As the temperature of the sample is increased the weak localization correction diminishes signifying a reduction of $l_\phi$ due to a loss of coherence in the sample, presumably due to electron-phonon interactions. Nevertheless it is important to note that the sample maintains a degree of coherence even up to 75 Kelvin.

3.3 Disorder Induced Interference

The weak localization effect examined in the previous section illustrate that the transport in our NWFETs maintains a significant degree of coherence at low temperatures and is therefore subject to quantum interference phenomenon. In one-dimensional channels, scattering from ionized impurities can multiply scatter carriers resulting in interference between the propagating wave packets. This interference degrades the smooth conductance plateaus expected in the ideal one-dimensional channel and obscures the underlying sub-band structure.

Disorder induced interference in one-dimensional nanostructures has been well documented in long-channel QPC structures$^{47-49}$ and more recently in VLS grown nanowires$^{36,50}$ where researchers have observed significant distortion from the ideal step-structure expected in the conductance. Numerous theoretical studies have simulated the effect of coherent scattering in the channel and shown the sign, strength, location and profile of the potential contributions from impurities will directly affect the lineshape of the conductance spectrum with different configurations
leading to dips, peaks, oscillations and in the case of large disorder completely extinguish any semblance of a step structure.\textsuperscript{51-55}

In general, the exact potential profile throughout the channel will determine the overall scattering matrix and the resulting interference process.\textsuperscript{15} Accordingly, the specific arrangement of surface charges will determine the conductance lineshape. Not only is the location of these charges sample specific but their occupation/charge state will be stochastically dependant on the gate potential. This gives rise to a dynamic $G$ vs $V_g$ relationship whereby the conductance lineshape will be coloured by an evolving impurity configuration.

![Conductance spectra](image)

Figure 3.3: Conductance spectra for an InAs NWFET under different biased cooldown conditions. The lineshapes display significant variations for different thermal and electrostatic histories.
In spite of disorder, retrieval of ideal conductance quantization may be possible under certain conditions. Numerical work by Laughton et al.\textsuperscript{53} illustrated that the major cause of quantization degradation in disordered 1D systems are so called “dips” in the channel potential which form quasilocalized states and create an indirect means of back-scattering. In the absence of such back-scattering mechanisms, retrieval of perfect conductance quantization was predicted. Put another way, a unimodal potential profile will restore conductance quantization in a one dimensional channel and eliminate resonant interference effects.

In Figure 3.4 the measured differential conductance for a HfO$_2$ capped sample under different electrostatic histories is shown. Typically, the device shows some signature of conductance quantization obscured by resonances and broadening due to scattering. The exact lineshape of the conductance profile is intrinsically linked to the specific interface charge configuration along the length of the channel. As the configuration of interface states depends on the gate bias history, significant variations in the conductance profile can occur as illustrated by the three blue traces. Electrostatic manipulation of surface charge state configurations result in a quenching of the interference (black trace) enabling observation of a perfectly quantized conductance spectrum.
Figure 3.4: Evolution of conductance vs gate voltage depending on electrostatic history. Experimental conductance values are scaled by the height of the first conductance plateau of 0.16$G_0$. The threshold voltages for all traces are nearly the same (~1.4V) but the curves are shifted horizontally for clarity.

In the absence of interference sub-bands transitions can be unambiguously determined from local maxima in $dG/dV_G$. The first six sub-bands are indicated in Figure 3.5 for the interference quenched nanowire.
Figure 3.5: Identification of the first six sub-band transitions from local maxima in dG/dV_g. The fifth and sixth sub-bands are approximately degenerate and therefore indistinguishable at 15K.

The ability to observe pristine stepwise conductance profiles in quantum point contacts enabled researchers to accurately pinpoint the band transitions in these systems. This ability to accurately probe the energy structure provided the foundation for an immense amount of progress in understanding the transport in these systems. Unfortunately, in the case of nanowires, the disorder inherent to their surfaces has been a limiting factor in obtaining clean transport and a review of the literature reveals an abundance of research founded on rather ambiguous data. Thus, the ability to quench this interference and observe clear band transitions is of
enormous significance and justifies a thorough investigation of the observed sub-band spectra. This will be a primary focus in the remaining chapters.
Numerical Models and Analysis

4.1 Introduction

In section 3.3 the linear conductance measurement for a NWFET exhibiting a remarkably clear step structure was presented. The absence of disorder induced resonances affords a clear window into the one-dimensional band structure of this device. Accordingly, data for this specific device will be the subject of comparison for subsequent models.

4.2 Carrier Density

The carrier density $N$ in the nanowire can be calculated by multiplying the distribution function by the wire’s density of states and integrating over energy.
Using the linear density of states yields the linear carrier density $N'$ in carriers per unit length

$$N'(E_F, T) = \int_{-\infty}^{\infty} f(\varepsilon)g(\varepsilon) \, d\varepsilon$$

$$= \int_{-\infty}^{\infty} \left( 1 + e^{\frac{\varepsilon - E_F}{k_BT}} \right)^{-1} \sum_n H(\varepsilon - E_n)D_n \frac{1}{\pi} \left( \frac{d\varepsilon}{dk_z} \right)^{-1} \, d\varepsilon$$  \hspace{1cm} (4.1)

To determine the carrier density at a given channel potential requires a summation across all sub-bands and integration across all energies. Repeating this calculation across a range of Fermi energies is computationally intensive; therefore it is advantageous to express the above equation in terms of the complete Fermi Dirac integral. This enables determination of $N'$ from pre calculated values in a Fermi integral table.

The step function can be removed from the expression above by switching the order of the integration and summation operations and changing the lower limit of the integration.

$$N'(E_F, T) = \frac{(2m^*)^{1/2}}{\pi \hbar} \sum_n D_n \int_{E_n}^{\infty} \frac{(\varepsilon - E_n)^{-1/2}}{1 + e^{\frac{\varepsilon - E_F}{k_BT}}} \, d\varepsilon$$  \hspace{1cm} (4.2)

The complete Fermi-Dirac integral of order $j$ is defined as

$$F_j(\eta) = \frac{1}{\Gamma(j + 1)} \int_0^{\infty} \frac{t^j}{1 + e^{t - \eta}} \, dt$$  \hspace{1cm} (4.3)
Where $\Gamma$ is the well known Gamma function defined by $\Gamma(j) = \int_0^\infty x^{j-1}e^{-x} \, dx$. Letting $t = \frac{\varepsilon-E_n}{k_B T}$ and $\eta = \frac{E_F-E_n}{k_B T}$ gives

$$N'(E_F, T) = \frac{(2m^*k_B T)^{1/2}}{\pi \hbar} \Gamma(1/2) \sum_n D_n \int_0^\infty \frac{1}{\Gamma(1/2)} \frac{t^{-1/2}}{1 + e^{t-\eta}} \, dt \quad (4.4)$$

The integral in the expression above is simply the complete Fermi-Dirac integral of order $-1/2$ thus $N'$ can be expressed as

$$N'(E_F, T) = \left(\frac{2m^*k_B T}{\pi \hbar^2}\right)^{1/2} \sum_n D_n F_{-1/2}(\eta) \quad (4.5)$$

### 4.3 Modeling the Capacitance

The capacitance of the device was calculated by relating the charge induced on the nanowire to the gate potential via Poisson’s equation

$$\nabla \cdot (\varepsilon(x, y)\nabla V(x, y)) = \rho(x, y) \quad (4.6)$$

Where $\varepsilon$ is the dielectric permittivity, $V$ is the electrostatic potential and $\rho$ is the charge density.

This differential equation was solved by employing finite element software (COMSOL Multiphysics). The dielectric constant of the SiO$_2$ region was taken to be $3.9\varepsilon_0$ and the HfO$_2$ region was taken to be $15\varepsilon_0$. The nanowire was modelled as a metallic conductor which is a reasonable assumption for InAs nanowires since they are
For a nanowire with a cylindrical cross-section and radius of 30nm, the capacitance per unit length was found to be $9.45 \times 10^{-11} \text{ F/m}$.

![Electric potential map](image)

Figure 4.1: Electric potential map for the cylindrical nanowire FET with a back-gate potential of 1V. The perimeters of the various gridding regions are outlined in black.

### 4.4 Relating the Gate Potential to Energy

The relative position of the Fermi level in the nanowire structure can be controlled by adjusting the potential of the back gate electrode. As the gate potential is varied the number of charges in the nanowire channel will change and the relative position of Fermi level with respect to the conduction band will shift accordingly. For a given change in the gate potential, the total change in charge will be proportional to the capacitance as illustrated in equation (4.7) below.

$$\Delta V_G = \frac{\Delta Q_{\text{Total}}}{C'}$$  \hspace{1cm} (4.7)
Where $C'$ is the capacitance and $Q'$ is the charge per unit length. It is important to note that the total charge induced will fill propagating states in the wire itself, as well as localized states at the surface. That is, $\Delta Q'_{\text{total}} = \Delta Q'_{NW} + \Delta Q'_{SS}$. Since $\Delta Q'_{NW}$ and $\Delta Q'_{SS}$ are both energy dependant quantities it is possible to relate the energy in the channel to the gate potential via $\Delta Q'_{NW} = e\mathcal{N}'(E, T) - e\mathcal{N}'(E_o, T)$ where the carrier densities $\mathcal{N}'$ can be calculated from equation (4.5) once the sub-band energies are known and $\Delta Q'_{SS} = eD'_{SS} \times [E - E_o]$ assuming a uniform density of surface donor states $D'_{SS}$ with respect to energy.

We define the threshold voltage $V_T$ as the gate potential at which the Fermi level is aligned with the first sub-band minima since this corresponds with device “turn-on”. With this formalism established $V_o = V_T$ and $E_o = E_1$ equation (4.7) can be expressed as

$$V_o = \frac{e(\mathcal{N}'(E, T) - \mathcal{N}'(E_1, T) + D'_{SS} \times [E - E_1])}{C'} + V_T$$

4.5 Conductance

In this section we utilize the theoretical framework outlined in the previous sections to model the $G$ vs $V_G$ expected for the wire of interest assuming a cylindrical cross-section. First, the sub-band minima $E_n$ and degeneracy factors $D_n$ are determined by solving the Schrodinger equation for a cylindrical hard wall potential. The radius of the cylinder was taken to be 30 nm as confirmed by SEM images of the NWFET. These values are implemented in the Landauer formula for the differential
conductance in a one-dimensional channel. Since the Landauer formula expresses the
differential conductance in relation to the chemical potential, a conversion to back
gate potential is performed via equation (4.8) which utilizes carrier densities
calculated from equation (4.5) and the capacitance which was determined via finite
element simulations. The density of surface states remains a free parameter in this
model since it will vary wire to wire and cannot be empirically determined by
conventional C-V spectroscopy because of the tiny gate capacitances inherent to
nanowires. Accordingly, the surface state distribution is assumed to be uniform in
energy where a density of $6 \times 10^{12} \text{ cm}^{-2} \text{ eV}^{-1}$ provides a good correspondence
between the modeled and measured $G \text{ vs } V_G$ trace which is consistent with estimates
of the surface state densities in the $10^{12} - 10^{13}$ range for InAs$^{36,37}$.

The simulated $G \text{ vs } V_G$ relation for a cylindrical nanowire agrees reasonably well with
the experimental data however there are some discrepancies. In the case of a
nanowire with a cylindrical cross-section, the second and third as well as the fourth
and fifth sub-bands are degenerate, that is sub-band minima $E_2 = E_3$ and $E_4 = E_5$.
This corresponds with twofold steps in the differential conductance as the Fermi level
crosses these sub-band minima. In the case of the experimental $G \text{ vs } V_G$ trace the
degeneracy between the second and third sub-band is slightly lifted, and there is a
significant lifting between the fourth and fifth sub-bands. These discrepancies
indicate a deviation from a cylindrical confinement potential and will be investigated
in the following chapters.
Figure 4.2: Conductance spectra of the measured device compared to simulation assuming a cylindrical hard-wall confinement potential
Morphological Band Structure Effects

5.1 Regular Hexagonal Cross-section

Up to this point, the sub-band structure of the InAs nanowire of interest was modelled under the assumption of it having a cylindrical cross-section. This is the assumption commonly made in literature since it has the practical advantage of estimating the band structure analytically. In reality, the cross-section of InAs nanowires are typically hexagonal. In view of this, the sub-band energies were recalculated under the assumption of a regular hexagonal cross-section in hopes of explaining the specifics of the observed band structure (the term “regular” is used here to indicate a hexagon which is both equilateral and equiangular). To do this the effective-mass Schrodinger equation was solved for a hexagonal hard wall potential. In contrast to the cylindrical case, there is no analytic solution to this differential equation with hexagonal boundaries. Accordingly, the eigenenergies were determined
numerically by employing a finite-element analysis software (COMSOL Multiphysics). The results for the first 10 sub-bands are summarized below in Figure 5.1.

Figure 5.1: Calculated sub-band minima for a nanowire with a circular cross-sectional geometry of radius $r=30\text{nm}$ and a hexagonal cross-sectional geometry with equivalent area

The results for the circle and the hexagon are nearly identical for the first 6 sub-bands. Most importantly, in the case of the hexagon the second and third as well as the fourth and fifth eigenstates remain degenerate, just as in the circular case. In fact it isn’t until the seventh and eight sub-band where the energy levels begin to deviate.

It is clear from these results that the confinement induced by a regular hexagonal cross-section cannot explain the anomalous band structure in this wire of interest.
Nevertheless, InAs nanowires and Wurtzite/Zincblende wires in general, are known to exhibit deviations from the regular hexagon morphology which would alter the electronic structure. High resolution scanning electron micrographs of vertical wires on the growth substrate confirm that some of our wires indeed exhibit such deviations.

![Figure 5.2](image)

Figure 5.2: High resolution scanning electron micrographs of InAs nanowires on growth substrate. (a) Nanowire exhibiting “regular” hexagonal morphology. (b) Nanowire exhibiting a “stretched” hexagonal morphology

### 5.2 Deviations from the Regular Hexagon

In this section we investigate the affect of morphological deviations from the regular hexagon on the one-dimensional electronic band structure. We begin by examining the effect of a “stretching” deformation, whereby the two opposing sides of the regular hexagon are elongated while keeping all angles between facets equal. This deformation is illustrated in Figure 5.3, with the two elongated facets denoted by length $a$, and the four shorter facets denoted by length $b$. The overall shape of the
cross section is defined by the ratio of the two lengths which we denote \( \zeta = \frac{b}{a} \). To investigate the effect of this deformation on the bandstructure, the first 10 sub-band minima are calculated by solving the Schrodinger equation under the effective mass approximation for cross-sectional geometries with \( \zeta \) values ranging from 1 to 0.3. The results of the simulations are given in Figure 5.3 and demonstrate the dramatic effect of morphological variations on the band structure of NWFETs. In view of this, a thorough characterization of the morphology for the nanowire of interest was performed and is outlined in the following section.

![Diagram of hexagonal cross-sections](image)

**Figure 5.3:** Dependence of the first ten sub-band minima on geometric anisotropy factor \( \zeta \) for hexagonal cross-sections with areas equal to that of a circle with radius \( r=30\text{nm} \)
5.3 Characterizing the Cross-sectional Morphology

To characterize the cross-section of the nanowire of interest, two approaches were taken. First, the nanowire was ruptured by joule heating, and the cross-section was imaged via high resolution scanning electron microscopy (Hitachi SU3500). The micrographs were taken at an angle of incidence which was in line with the wire’s longitudinal direction and an elevation of $20^\circ$ from the substrate plane. The perspective distortions at this angle of incidence were minimal, yielding images with vertical dimensions of $\cos 20 \approx 0.94$ of the true dimensions. The micrographs (Figure 5.5a,c) reveal a strongly irregular cross-sectional morphology for the NWFET. The SEM images provide a good general picture of the cross-sectional geometry however some of the facets are obscured by Hafnia, especially in the upper right portion where a bubble was generated in the joule heating process (see blue arrow in Figure 5.5c).

In order to more accurately characterize the cross-sectional morphology a more sophisticated approach was adopted which employed a Focused Ion Beam (FIB) system to remove a cross-sectional slice of the sample and thin it to electron transparency in preparation for imaging via Transmission Electron Microscopy (TEM).
Focused Ion Beam Systems

Much like SEM and EBL technologies, focused ion beam systems emit particles from their source and focus them into a highly collimated beam which can be manipulated by deflection coils scanned across a sample. In the case of FIBs, these particles are ions (most commonly Ga\(^+\)) and as these high energy particles impede on the sample they sputter material from the surface. At low primary beam currents the amount of sputtered material is small, enabling the system to perform relatively non-destructive imaging through detection of the ejected atoms. At higher beam currents, the sputtering rate can be drastically increased and the FIB behaves as a high precision mill. In addition FIB systems are capable of site specific ion beam mediated CVD deposition whereby specially selected precursor gases such as tungsten hexacarbonyl (W(CO)\(_6\)) can be introduced into the chamber and allowed to adsorb on the samples surface. As the ion beam scans over the surface the gas will disassociate freeing the volatile organic ligand and leaving behind the non-volatile component as a deposit on the surface.

FIB Microsampling and TEM Characterization

In this work, a state of the art dual beam FIB-SEM (Hitachi NB5000) was utilized to perform a microsampling/lift-out process whereby a microscale section of the sample containing the nanowire of interest was removed from the bulk and transferred to a TEM half grid. The microsample is then thinned to electron transparency (~100nm) to form a suitable lamellae for TEM imaging of the wire’s cross-section. The microsampling process is outlined below:
First, a layer of Tungsten (W) is deposited over the region of interest to form a protective barrier to ion implantation damage during subsequent milling procedures.

Deep vertical trenches are milled around the perimeter of the area of interest save for a small tab which remains connected to the bulk substrate. Subsequent mills are performed at an angle to undercut the coupon and free the base from the bulk.

A motor controlled probe known as a micromanipulator is brought in contact with the coupon and affixed to the surface via Tungsten deposition.

The connecting tab is milled away and the free microsample is lifted out with the micromanipulator and affixed to a TEM sample holder via Tungsten deposition.

Once the coupon is secured to the grid the tip of the micromanipulator is milled away, freeing it from the sample. The microsample is then thinned to electron transparency with the ion beam in preparation for TEM imaging.
Figure 5.4: FIB microsampling process. (a) Vertical trenches are milled around the area of interest, defining the perimeter of the coupon. (b) Angled mills undercut the coupon and free the base from the bulk substrate. (c,d) Micromanipulator is brought in contact with the coupon. (e) Micromanipulator is affixed to coupon by tungsten deposition. (f) Connecting tab is milled away, freeing the coupon from the substrate. (g,h,i) Coupon is lifted out from the substrate and brought in contact with the TEM grid. (j) Coupon is affixed to the TEM grid via tungsten deposition. (k) Tip of micromanipulator is milled away, freeing it from the coupon. (l) Coupon is milled to electron transparency, forming a suitable lamellae for TEM imaging.
In Figure 5.5b below a TEM image of the NW cross-section is shown with facets outlined in yellow. This geometrical fit from the TEM image of the cross-section under the contact is overlaid atop the SEM image of the cross-section at the center of the wire in Figure 5.5c and illustrates that the morphology remains constant along the length of the wires.

![Figure 5.5: (a) Angled SEM image of the ruptured NW. The HfO2 regions are coloured yellow and the source/drain contact is coloured brown. The FIB cross-sectional slice was taken from a region of the wire under the Ti/Au contact as indicated by the dashed line. (b) TEM image of the FIB milled NW cross-section. The Ti/Au contact region is indicated in brown colour. The NW cross-section geometry is outlined by the yellow trace. (c) SEM image of the ruptured NW cross-section. The cross-sectional geometry obtained from FIB/TEM characterization (yellow trace) is overlaid atop the SEM image. The excellent agreement indicates that the NWs geometry remains constant along the length of the wire. A HfO2 bubble which was generated in the rupturing process obscures the upper-right most portion of the NW face and is indicated by the blue arrow.](image)

Further characterisation by selective area diffraction (SAD) yields diffraction patterns indicative of growth in the [211] direction which helps to explain the peculiar cross-sectional morphology of the wire of interest. Although growth of InAs nanowires
tend to propagate in the [111] or [0001] directions, propagation in the [211] direction has been reported by various authors\textsuperscript{58}.

5.4 Structural Confinement Effects from Observed Morphology

Utilizing the geometry obtained from TEM microscopy, the Schrodinger equation was solved for hardwall boundaries defined by the geometry outlined in Figure 5.5. The resulting sub-band spectrum for the first 6 sub-band modes is displayed in Figure 5.6 and the wavefunctions for each subband mode are shown in Figure 5.7. It is apparent from the large discrepancy between the experimentally observed band structure and that defined purely by the structural confinement that there are additional contributions to the confinement potential. These contributions will be explored in the following chapter.
Figure 5.6: (a) Sub-band energies for a hard-wall confinement potential defined by the characterised cross-sectional geometry of the nanowire. (b) Ballistic conductance spectrum for this morphology at 15K
Figure 5.7: Wavefunctions for the first six sub-bands assuming a hard-wall confinement potential defined by the observed cross-sectional geometry.
Electrostatic Influence on Sub-Band Structure

Up to this point, electrostatic contributions to the confinement potential have been neglected and it is evident from the large discrepancy between the observed sub-band spectrum and that predicted purely by structural confinement, that these electrostatic contributions are significant. Such electrostatic contributions likely arise from ionized interface states which are known to play a significant role in semiconductor devices, especially in the case of nano-structured devices because of their extremely large surface to volume ratios.

InAs in particular is known to have a large density of donor like surface states located above the conduction band edge resulting in large densities of positively charged ions at the surface\textsuperscript{59,60}. Nevertheless, it has been shown that high-k dielectrics such as HfO\textsubscript{2} can passivate these states\textsuperscript{61,62} and accordingly the density of ionized donors is expected to be greatly diminished at HfO\textsubscript{2}-InAs interfaces. For the structures studied in this work the HfO\textsubscript{2} is absent from the bottom interface of the
nanowire and therefore a large anisotropy of charged surface states is expected which would have a significant impact on the confinement potential.

The recovery of six band transitions in the interference quenched device, serves as a robust fingerprint of the energy structure in the nanowire. Given that the geometry of the nanowire has been fully characterized, the structural contributions to the confinement potential are known and therefore it should be possible to deduce the electrostatic contributions from the interface states. In this way the relative densities of the interface states may be mapped directly from the conductance spectrum. Such a process would involve self consistently solving the Schrödinger and Poisson equations and will be the focus of future work.
Conclusions

This thesis investigated electronic transport in nanowire transistors in a regime where ballistic transmission and quantum confinement play significant roles. It is our hope that the experimental findings and critical analysis will help to advance the burgeoning field of quantum electronics.

Investigations of quantum interference phenomena in various nanowire transistors illustrated the significant role of disorder on the conductance spectra and its limiting effect on achieving ballistic conduction, as evidenced by the breakdown of conductance quantization. It was shown that the potential landscape of nanowire transistor channels could be altered by electrostatic manipulations of surface charge state configurations thereby modifying the resulting interference process. We have demonstrated that such manipulations can result in a complete quenching of the disorder induced interference, resulting in perfect quantization of the ballistic
conductance. This finding is of great significance, as perfect quantization of numerous sub-bands had yet to be realized in nanowire structures.

Furthermore, the quenching of the quantum interference in the nanowire transistor eliminated distortions in the conductance spectra, enabling direct insight into the one-dimensional band structure. The recovery of six sub-band transitions served as a robust fingerprint of the confinement potentials and numerical models illustrated a deviation from cylindrical hard-wall confinement in the nanowire of interest.

Simulations investigating the role of morphological variations demonstrated a strong affect on the band structure of one dimensional quantum structures, prompting thorough morphological characterization of the interference quenched nanowire. Focused ion beam lift-out techniques were employed to remove a cross-sectional slice of the nanowire, enabling accurate characterization via transmission electron microscopy. Numerical models adopting the characterized morphology under hard-wall confinement potentials demonstrated a large deviation from the measured sub-band spectrum and point towards significant electrostatic contributions to the confinement potential from ionized interface states.

Finally, we discuss the possibility of utilizing the observed sub-band spectrum as a means of probing the interface state densities. This process could provide spatial resolution of interfacial charge densities, something which is not possible with conventional capacitive techniques.
Bibliography


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