ARRAYS OF SILICON P-I-N NANOWIRES FOR ANTENNA-ENHANCED AND POLARISATION SENSITIVE DETECTION OF LIGHT

by

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Abstract

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A novel antenna effect is demonstrated in arrays of 500, 200 and 100 silicon nanowires embedded in silicon dioxide. The silicon nanowire gratings are analyzed using spectral and polarisation resolved photocurrent microscopy. Resonant enhancements in the electric field and thus photocurrent response are observed at multiple wavelengths corresponding to coupling of incident radiation into the grating’s multiple-scattering electromagnetic modes. The photoresponse retains the sinusoidal polarisation anisotropy expected in single nanowires. The resonances are modeled quantitatively using electromagnetic scattering theory and show excellent agreement with measurement. A experimental quality factor of $Q \approx 10$ was measured for the gratings, exceeding that of a single wire, but lower than expected from theory which gives $Q \approx 70$. The difference can be ascribed to the finite length of the wires and their termination at ohmic contacts. Strategies to improve $Q$ are discussed, and a polarisation sensitive grating is presented to resonantly enhance light detection at red, green and blue wavelengths for application as a colour imaging sensor.
Dedication

To my family.
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Chapter 1

Introduction

Since the dawn of the 19th century, the light-matter interaction and the field of photonics in general has been studied with intense interest and is the bane of many modern technologies, including the development of lasers, sensors, light emitting diodes, solar panels, and fibre-optic communication [2, 3]. With increasing interest in reducing power consumption, extending component lifetime and studying physical phenomena at the nanoscale, it’s obvious that the miniaturization of components which make up these devices will continue to be of paramount importance [4]. Much of these existing technologies are based upon bulk or thin film semiconductors, typically on silicon based platforms, which suffer from considerable loss due to reflection, poor signal-to-noise ratios and often bulky physical dimensions [5, 6]. In order to move forward, the constituents that make up these devices must be drastically reduced in physical dimension, yet must still be compatible with existing silicon based technologies.

Compound semiconductor homostructures and heterostructures are becoming increasingly prevalent as a solution to further enhance and understand the interaction between light and matter [7]. Semiconducting nanowires, nanopillars and quantum dots are some of the most popular, reproducible nanostructures that are suitable for manipulating and utilizing the light-matter interaction to our benefit. The focus of this thesis will be
Chapter 1. Introduction

on optical sensing, in particular for the detection of visible wavelength radiation, using semiconducting nanowires.

Nanostructured materials, and particularly nanowires, are of interest in these applications for many reasons including ease of integration with current silicon electronics due to their small dimensions, and fabrication flexibility in terms of substrate and environment [6]. The detection of photons is necessary for imaging, spectroscopic applications and fibre-optic communication. Current visible wavelength technology is based on bulk silicon detectors and suffers from several drawbacks including [3],

- Weak absorption over the entire visible and infrared spectrum of radiation
- Long interaction lengths required for high sensitivity
- Interfacial lattice mis-match issues resulting in defective optical properties
- High mobility and long diffusion lengths/lifetimes leading to cross-talk between pixels and blurring of optical signals at smaller pixel sizes

The goals to be achieved by developing sensing technologies using nanowires will be to expand the absorption spectrum, minimize physical dimensions and volumes of materials required and amplify signals by minimizing noise and enhancing responsivity.

1.1 Semiconductor Nanowires

Semiconducting nanowires are inherently one or quasi one-dimensional semiconducting structures (depending on their diameter and material properties) with drastically larger surface-to-volume ratios than their thin film counterparts. Nanowire growth can be grouped into two categories, bottom-up and top-down growth, the latter being the mechanism by which the samples presented in this thesis were created.

Bottom-up growth is based on the vapour-liquid-solid (VLS) growth mechanism first proposed by Wagner and Ellis, and involves chemically synthesizing nanowires [8]. Briefly,
the nanowires are formed when the desired nanowire material is adsorbed from its gaseous phase onto a metallic, liquid catalyst (such as gold) as it grows vertically. This particular approach provides a natural mechanism for growing dislocation-free, single crystalline nanowires \cite{8} implying fewer dangling bonds at the surface of the nanowire, giving good control over surface state density and thus carrier density \cite{9}. Furthermore, this method provides a natural mechanism for relaxing lattice strain at interfaces and can allow for a variety of structures on lattice mismatched substrates \cite{10}, allowing for the possibility of growing more exotic nanowires that are not available in bulk form \cite{9}. Due to the fact that these nanowires are produced in dense, randomly oriented ‘forests’, their feasibility for high density, aligned nanostructures is limited in comparison with top-down grown nanowires \cite{9}.

Top-down growth typically involves etching and oxidizing material from a bulk wafer substrate, defining the specific nanowire geometries using a technique such as optical or electron beam lithography \cite{11}. This technique is diffraction limited and the feature size is a linear function of the wavelength of the incident radiation \cite{9}. Top-down growth allows for superior control over placement of nanowires and feature size and is well suited for defining arrays of nanowires \cite{9}, in particular the nanowires presented in this thesis \cite{11}.

Nanowire’s unique size and shape allows for the possibility to integrate more inherent functionality into photonic devices, using homo or heterostructures. Although their optical properties are largely dependent on the dielectric properties of bulk materials, many interesting properties emerge due to their unique structure including polarisation sensitive effects which will be discussed in more detail in Chapter 3. Nanowires have shown promise in a multitude of applications including gas sensing \cite{12,13}, nanowire lasing \cite{14,15}, biological sensing \cite{16,17}, use as logic gates \cite{18} and have even shown promise for quantum computing as a spin qubit in a nanowire has been experimentally demonstrated \cite{19}. An additional advantage to using nanowires as building blocks in photonic devices is the possibility of exploiting their non-linear properties \cite{20}.
1.2 Objectives

The main aim of this thesis is to explore the realization of a multi-nanowire based photodetector, in which we can simultaneously minimize the physical dimensions of the device, while drastically increasing the responsivity and signal-to-noise ratio of the detector as a platform for the detection of visible radiation.

Given the large surface-to-volume ratio inherent to nanowires, they have a natural mechanism to reduce noise generated by dark current due to their small volume. This also has the advantage of reducing the volume of material required as well as lowering power consumption. Responsivity is also enhanced by utilizing collective light scattering effects from the array of nanowires. I will show that by thoughtful choice of the size of the individual nanowires and the pitch of their periodic spacing it is possible to engineer resonant enhancements into the optical absorption spectrum of the device.

Though nanowires are an attractive alternative to planar, thin film based semiconductor devices, they are necessarily more complicated and as such it is desirable to get the most functionality and efficiency possible out of each device. One of the biggest hurdles nanowire technology has yet to overcome is the reliable scalability and reproducibility of manufacturing said devices. The top-down grown nanowires presented in this thesis have the advantage over bottom-up nanowires in that it is possible to produce large arrays of nanowires with consistent, small feature sizes. Though lacking the inherent crystallinity and engineered facets of bottom-up nanowires, they have an advantage in reproducibility due to the fact that the same mask used to define the wires in the lithography process may be used repeatedly.

1.3 Optical Sensing Overview

Nanostructured materials, and in particular nanowires, are an attractive alternative for optical sensing compared to their thin film counterparts for a variety of reasons, including
their ease of integration with current silicon electronics and large surface-to-volume ratio. There are a wide variety of possible schemes for detecting photons using nanostructures, and though they differ in the physical mechanism by which they generate an electrical signal, there are common figures of merit for photodetectors by which to benchmark individual device performance,

- **Responsivity** $R$ [A/W]: This is a measure of optically induced current (or electrical output) flowing through the device as a function of incident optical power. Responsivity is a function of wavelength, dielectric properties, and device geometry and must be well defined for proper use of any photodetector.

- **Gain** $g$ [-]: Gain is the ratio of the photocurrent, or the number of photo-generated electrons per second [$\#e/s$], to the number of photons absorbed. If there is one electron-hole pair created upon absorption of one photon in the photodetector the gain is unity.

- **Dark Current** $I_d$ [A]: Current flowing through a device in the absence of light is referred to as dark current. Possible sources include the release of trapped carriers, or thermally generated carriers, which are swept to the contacts by the built-in-field registering a signal.

- **Quantum Efficiency** $QE$ [%]: Quantum efficiency (QE) is the ratio of photocurrent [$\#e/s$] to photons incident [$\#\text{phot.}/s$], a measure of the percentage of photons hitting the active area of the photodetector that produce charge carriers, and is often a function of incident optical wavelength.

Using nanowires as photodetectors is a well understood concept and the field has gained much attention in the last several decades. Significant research has been pursued using directly grown nanowires as photodetectors including the use of InAs nanowires, Si nanowires, GaAs nanowires, CdSe nanowires, and a Si...
nanowire phototransistor \[25\]. More complex devices for photon detection have been realized using transfer printing including GaN nanorod p-n junctions \[26\], core-shell CdSe/CdS nanorods \[27\], and crossed Ge/CdS nanowire heterojunctions \[28\]. There has also been much interest in oxide based, ZnO nanowire based photodetectors \[29\], and plasmonic nanowire photodetectors \[30\].

These detectors all generate electrical signals based on the absorption of incident radiation promoting an electron to the conduction band to create so-called photo-generated carriers, which are absorbed into a collection circuit, but there are three principle classes of nanowire photodetectors including photodiodes, photoconductors and phototransistors, which I will describe briefly.

**Photoconductor**

Photoconductors are simply slabs of semiconductor situated between two ohmic contacts. When photons of sufficient energy impinging on the semiconductor are absorbed, an electron-hole pair is created. The resulting increase in carrier concentration within the structure subsequently increases the conductivity of the device, which is measured by a read-out circuit. Photoconductors are very simple, rugged structures and have inherently high values of gain \[31\] due to the fact that one charge carrier is often trapped by either a surface state, ionized impurity or donor/acceptor state, allowing the complementary carrier to circulate through the device multiple times before recombining \[32\]. The main drawback to photoconductors is the inherent trade-off between gain and speed due to the fact that when a significant population of carriers is introduced into the semiconductor the device takes a long time to recover to its nominal state.

**Phototransistor**

Phototransistors operate similarly to photodiodes, absorbing photons in the base-collector junction of the device to create carriers. The electrons flow from the emitter to the collector, and the subsequent current is amplified by the transistor resulting in increased gain and responsivity \[31\]. This contrasts avalanche photodiodes in that the need
a high voltage to increase gain is eliminated, thus significantly reducing the amount of 
noise. Again, the increased responsivity and complexity of the device comes at the cost 
of longer response times.

**Photodiode**

Photodiodes are typically P-N or P-i-N structures (such as the detection platform pre-
resented in this thesis [32]), in which the intrinsic or depletion region of the structure 
absorbs incident photons to create charge carriers. These devices operate under zero bias 
as the built-in electric field separates the charge carriers. As a result, unbiased photodiode 
as only capable of a gain of unity. Photodiodes are capable of very high speed 
operation by keeping device dimensions small, while quantum efficiency may be improved 
upon by increasing the depletion layer thickness [31]. P-i-N junctions have an advantage 
over P-N junctions in that the electric field in the intrinsic region is much higher, giving 
the device a faster response time due to the dominance of the drift process, which is 
much faster than the diffusion process more dominant in P-N junctions.

If operated at high reverse-bias voltages, photodiodes can enter the avalanche multi-
plication regime. At this high reverse-bias voltage the electric field is substantial enough 
to cause impact ionization of carriers, resulting in high values of gain from multiplication 
of carriers and increased responsivity [32], which differs from the mechanism of photo-
conductive gain described earlier. The multiplication factor characterizing this process 
is principally a function of depletion layer thickness and the carrier ionization rates. The 
drawback to avalanche photodiodes is the significant increase in noise associated with 
the high electric field in the depletion region, as well as slow response times due to con-
tinuous flow of current, though the response time can be considerably improved upon by 
implementing a quenching circuit [33].

Nanowire based photodetectors have numerous applications in photonics and will help 
pave the way to reducing not only the size of future electronics, but the ecological foot-
print. With the continuing advance from electrical to optical communication, nanowire
photodetectors may be used as optical interconnects on chip photoreceivers \cite{34}, being superior to current technology due to their potential for high internal gain, low noise and minimal power consumption. Furthermore, the need for reliable single photon detection is becoming increasingly apparent, and several nanowire based photodetectors have already shown considerable promise \cite{35,36}. In contrast to chemically grown nanowires, lithographically defined nanowires not only allow for dense and ordered spatial integration, but have the advantage in that they may be selectively addressed with minimal cross-talk between pixels \cite{3}.

1.4 Enhancement Schemes

There are several strategies for enhancing absorption in single and arrays of nanowire based photodetectors which are becoming increasingly prominent in detector design, including plasmonic enhancement, photon trapping in cavities, and resonant design of individual nanowires/nanowire arrays.

Plasmons are collective oscillations of electrons in a metal and are engineered into compound systems with nanostructures using metallic nanoparticles of various morphologies, most commonly spheres or rods. The enhancement is two-fold as the nanostructures not only experience increased absorption due to enhancement in electromagnetic fields at the surface of the metal particle, but optical waves may couple to these localized excitations, further enhancing absorption of radiation \cite{37}. The plasmonic interaction is fairly well understood in the sense that there is considerable control in engineering resonant frequencies using a variety of metals and nanoparticle morphologies, allowing for enhancements from the UV to the mid-infrared frequency range \cite{37}. Enhancement in absorption of radiation has been demonstrated in Si nanowires using gold nanoparticles \cite{38}, in GaAs solar cells using Ag nanoparticles \cite{39} and in Si photodiodes using Au/Ag core-shell nanorods \cite{40}. Owing to the fact that plasmonic enhancement is achieved through use of
metal nanoparticles, their application may be limited due to the lossy nature of metals as heat is always produced when radiation is absorbed or manipulated by metals.

Due to the ultra small diameter of nanowires, radiation transits the absorbing region of nanowire based devices very quickly, with only a small percentage of the total radiation being absorbed. In order to increase absorption in nanowires, an alternative to plasmonic enhancement is to trap photons in a cavity like structure. Cavities are simple in principle in that they confine light to a small, ideally sub-wavelength volume, subsequently increasing the lifetime of photons in close proximity to the nanowire, thus resulting in an increased absorption probability \[41\]. Cavities can be as simple as a planar anti-reflective coating on the surface of the nanostructure, with a highly reflective backing or substrate \[42,43\]. It is apparent from the Fresnel equations that reflection of photons can be readily achieved by dielectric contrast between the material which encapsulates the nanowires and the surrounding structure. Reflection coefficients are given by the Fresnel equations and are governed only by the incident angle of radiation and dielectric properties of the two materials at a particular interface \[44\]. By designing a cavity in such a way that the dielectric properties of the material surrounding the nanowires strongly contrast that of the surrounding cavity, total internal reflection can be obtained for a large variety of incident angles.

It is also possible to engineer resonances directly into individual or arrays of nanowires themselves. In this thesis resonant enhancement is achieved when collective scattering from the ordered array of nanowires and the cavity structure interferes constructively, forming a standing wave pattern in which electric field maxima can be observed at several wavelengths. However, it is also possible to achieve antenna-enhanced photoresponse in single nanowires by exploiting leaky-mode resonances \[45,47\], which occur in larger nanowires (often several hundreds of nanometers in diameter).

Leaky-mode resonances occur when nanowires are of sufficient size to act as a resonator and trap light in circulating orbits around the nanowire, due to multiple total
internal reflections from the periphery of the wire. These resonances are solutions to Maxwell’s equations and are characterized by azimuthal and radial mode numbers $m$ and $l$, corresponding to the effective number of wavelengths along the circumference and the number of radial field maxima within the nanowire respectively [45]. The resonances are leaky in nature because the fields extend outside of the wire and interact with the surrounding environment. To achieve enhancement in the visible wavelength regime relatively large diameter nanowires are required, as the resonance wavelength scales linearly with the diameter of the nanowire [45].

1.5 Photocurrent Spectroscopy

Photocurrent spectroscopy is a powerful tool that may be used to investigate the local electronic structure in nanoelectronic devices. By generating charge carriers in the structure by means of an optical excitation and measuring the short-circuit current produced, it is possible to determine properties of the electric field distribution in the region of interest. Photocurrent spectroscopy is a very popular, non-invasive method of probing the electric properties of nanostructures and has been used to examine silicon nanowire field effect transistors (FETs) [48], CdS nanowires [49], graphene based devices [50], and numerous other nanostructures.

At the heart of it, the physical property of the silicon nanowires (SiNWs) presented in this thesis that allows for them to be used for photodetection is the P-i-N junction. The SiNWs in this thesis are selectively doped in a P-i-N structure with phosphorus and boron to define N and P doped regions respectively. The intrinsic region between the two doped regions is $\approx 500$ nm in length. Figure 1.1 shows the energy band diagram for the P-i-N structure of each individual SiNW.

Due to the physical separation of charged dopants at either end of the nanowire, there is an inherent electric field that builds up across the intrinsic region of the P-i-N
Figure 1.1: Energy band level diagram for P-i-N nanostructure along the $\hat{z}$ direction showing transport of photogenerated electrons and holes upon absorption of a photon with energy $h\nu$. Energy levels are with respect to vacuum energy level $E_{\text{vac}}$, with conduction band, valence band and Fermi energy levels denoted as $E_c$, $E_v$ and $E_F$ respectively.

junction in each nanowire. A photon impinging on this intrinsic region with sufficient energy $E = h\nu$, equal to or above the band gap of silicon, may impact an electron and cause it to be promoted from the valence band to the conduction band of the nanowire. This is what may be referred to as ‘pair production’ as an electron can now be found in the conduction band, and subsequently a hole is left behind in the valence band, hence the ‘pair’.

The two photo-generated charges experience the built-in electric field in the intrinsic region of the P-i-N junction, and are subsequently separated, holes moving towards the anode and electrons towards the cathode. The total current flowing through the junction at any given moment in time is the sum of photocurrent generated by photo-excited carriers, and dark current due to thermally excited carriers.

1.6 Steady-state Carrier Dynamics

The rate of change in carrier concentration and hence the dynamical behaviour of charge carriers in a semiconductor is given by the continuity equations defined as follows,
\[ \frac{\partial p}{\partial t} = \frac{-1}{q} \nabla \cdot \vec{J}_h + G - R \] (1.1)

\[ \frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \vec{J}_e + G - R \] (1.2)

where \( G \) is the photo-generation rate of charge carriers, \( R \) is the recombination rate of charge carriers, \( p \) and \( n \) are the concentrations of positive and negative charger carriers (holes and electrons), and \( J_h \) and \( J_e \) are their respective current densities. Neglecting diffusion and assuming electrons and holes undergo an average time of \( \tau_e \) and \( \tau_h \) before undergoing recombination, the continuity equations can be reduced to,

\[ \frac{\partial p}{\partial t} = -\mu_h E \frac{\partial p}{\partial x} + G - \frac{p}{\tau_h} \] (1.3)

\[ \frac{\partial n}{\partial t} = \mu_e E \frac{\partial n}{\partial x} + G - \frac{n}{\tau_e} \] (1.4)

where \( E \) is the electric field present in the intrinsic region and \( \mu_h \) and \( \mu_e \) are the mobilities of holes and electrons respectively.

An important feature of Equations (1.3) and (1.4) is the fact that one can increase the rate at which the carrier concentration changes (and thus photo-generated charge carriers reach the contacts) by increasing the electric field across the intrinsic region of the junction. This is accomplished by applying a constant potential difference across the junction in what is known as ‘biasing,’ illustrated in Figure 1.2.

To operate the P-i-N junction in forward bias, a potential difference is applied across the junction connecting the positive and negative contacts of the junction to the positive and negative terminals of the power source respectively. This has the effect of causing the intrinsic region in the centre of the P-i-N junction to contract as the applied potential opposes the built in electric field, i.e. the holes in the P-type region and the electrons in the N-type region are pushed towards the junction. To reverse bias the junction the opposite has to happen, that is the positive and negative contacts of the junction are
Figure 1.2: Energy band level diagram for P-i-N nanostructure for forward, zero and reverse bias voltages. Conduction, valence and Fermi energy levels denoted as $E_c$, $E_v$ and $E_F$ with quasi Fermi energy levels for the P and N doped regions denoted as $F_P$ and $F_N$ respectively. The width of the intrinsic region over which the electric field is present is denoted for forward, zero and reverse biases as $W_F$, $W_0$ and $W_R$ respectively.
connected to the negative and positive terminals of the power source. This has the effect of pulling the holes in the P-type region and the electrons in the N-type region away from the junction, causing a much larger depletion region and increased electric field across the junction.

Photodiodes are often operated under reverse bias for two reasons. First, by operating under reverse bias one can increase the size of the depletion region, thus increasing the active area in which photons may be absorbed to produce electron-hole pairs. Secondly, when the junction is under reverse bias much higher electric fields may be obtained, subsequently decreasing the transit time photo-generated carriers undergo before reaching contacts, improving the response time of the photodiode. As mentioned earlier, when high enough reverse bias voltages are obtained it is possible to enter the avalanche multiplication regime in which a photodiode may experience gain \[32\]. The nanowire photodiode presented in this thesis is operated exclusively under zero bias.
Chapter 2

Experimental Results

The arrays of SiNWs presented in this thesis were fabricated by our collaborator at Nanyang Technological University in Nanyang, Singapore. The electron beam induced current measurements presented in Section 2.2 were obtained by Michael Chen, a fellow colleague at CAN. All other measurements were performed by myself.

2.1 Sample Preparation

The SiNWs were created using top-down fabrication on a silicon-on-insulator (SOI) substrate shown schematically in Figure 2.1 and described in detail elsewhere [51]. Briefly, 120 nm of Si was deposited as a top layer and using alternating phase shift mask lithography with a KrF scanner and patterned photoresist, parallel arrays of $N = 500, 200$ and 100 rectangular fins with a width of 120 nm were formed. After plasma resist trimming and silicon etching, the fins were reduced to a width of 45 nm, height 120 nm and length 1 $\mu$m. The fins were further reduced to ultra-small SiNWs by a dry oxidation process, resulting in a triangular cross-section.

The P-i-N doping profile was achieved by ion implantation of phosphorous ($\approx 10^{20} cm^{-3}$) and boron ($\approx 10^{20} cm^{-3}$) on opposite ends of the wire. The dopants were activated by annealing the wires at a temperature of 1000$^\circ$ C for 5 seconds. The intrinsic region was
Figure 2.1: Schematic of SiNW array fabrication process. Starting with a patterned photoresist (PR) and bottom anti-reflective coating (BARC), the resist is subsequently trimmed, silicon fins are etched, the resulting silicon fins are dry oxidized, which is then followed by ion implantation of phosphorus and boron to form the anode and cathode respectively. Copyright © 2008, IEEE (reprinted with permission).

estimated to be 500 nm in length through process simulation. After removal of the native thermal oxide by etching in Hydrofluoric acid (HF), the SiNWs were encapsulated in a 550 nm thick layer of SiO$_2$.

Cross-sectional transmission electron microscopy (TEM) was used to examine the post-processed SiNWs, shown in Figure 2.2B. One can see they have a triangular cross-section with base width $w \approx 6$ nm and height $h \approx 8$ nm. The SiNWs sit 150 nm above the Si/SiO$_2$ interface of the SOI substrate and are surrounded by SiO$_2$, as can be seen in a schematically in Figure 2.2A. The roundness of the triangular cross-section can be attributed to the non-ideal aspect ratio of the pre-oxidized fins.

2.2 Electron Beam Induced Current

In order to confirm that the intrinsic region of the SiNWs is indeed the region responsible for the short-circuit photocurrent generation, the junctions were imaged using electron-beam-induced-current (EBIC) using a low-noise current preamplifier in a scanning
Chapter 2. Experimental Results

Figure 2.2: A. Schematic illustration of Si P-i-N nanowire (SiNW) structure embedded in 550 nm thick SiO$_2$ layer located upon a silicon substrate. The stars denote photo-generation of electron-hole pairs in the intrinsic region along with their direction of diffusion towards the heavily doped contacts (not shown) as indicated by arrows. B. Cross-sectional TEM image of SiNW embedded in SiO$_2$ with base width $w \approx 6$ nm and $h \approx 8$ nm (scale: 10 nm).

electron microscope with a 15 kV acceleration voltage. Shown in Figure 2.3A, one can see the bright, central regions responsible for producing electron-hole pairs that are subsequently collected by the cathode and anode respectively. The P and N doped regions, as well as the heavily doped contacts, do not exhibit a photocurrent response as there is no built in electric field aiding in the collection of charges.

A line scan of the EBIC profile as shown in Figure 2.3B allows for an accurate estimation of the effective junction length $L$ required later in the determination of responsivity $R$ of the structure from photocurrent measurements. The length of this region is estimated to be $L = 470 \pm 50$ nm from the line profile. In Figure 2.3B one can see the highly doped P and N regions on either side of the junction do not contribute to short-circuit current and match the dark regions present in Figure 2.3A as expected. These measurements confirm the approximate doping profile P(250 nm)-i(500 nm)-N(250 nm) expected from process simulation. The bright regions in the cathode and anode regions labeled in Figure 2.3A is produced by a direct charge injection mode, called resistive EBIC [52].

The negative EBIC signal measured in the P and N type regions of the SiNWs occurs due to direct injection from the electron beam outside the region of the built-in
Figure 2.3: A. Electron-beam-induced-current (EBIC) image showing SiNWs connected in parallel to cathode and anode electrodes. Bright central regions in SiNWs are responsible for generation of electron-hole pairs producing a short-circuit current (scale: 1 µm). B. EBIC line profile of a single SiNW in the grating showing.

field [52, 53]. An electron directly injected into the P region would immediately recombine, creating a current flow from the anode which would be in opposition to the current generated by an electron-hole pair in the junction. Similarly, if an electron was generated in the cathode it could recombine with an excess hole from the P region, producing the same response. From Figure 2.3A we can see the EBIC image is blurred in appearance. This is due to a stochastic interaction between the electron beam and the SiO₂ material, causing the electron beam to spatial broaden 400 nm below the SiO₂ surface where the SiNWs are located, making the SiNWs appear to exceed their physical width [52].

2.3 Photocurrent Measurement Apparatus

Short circuit photocurrent measurements were performed for excitation wavelengths of 400 < λ < 700 nm for the 500, 200 and 100 SiNW gratings. No external bias was applied to the gratings. Optical excitation was provided using a combination of a broadband halogen bulb light source and an optical spectrometer, which after collimation was focused on the sample stage at normal incidence using an objective lens. An adjustable aperture was used to control the area of the illuminated area and the excitation was gated using an electro-mechanical shutter. Polarizing plates allow control over the orientation of the
polarisation of the optical beam and measurements were performed for both polarized and unpolarized excitation. Polarisation can be obtained for any arbitrary polarisation relative to the SiNW axis.

Figure 2.4: Schematic of experimental optical setup including halogen lamp, optical spectrometer, aperture, moveable beam-splitter (BS) for imaging the illuminated are of sample on CCD, final objective lens, and chip carrier.

The diced chips containing the SiNWs were wirebonded in chip carriers as shown in Figure 2.5B. These chip carriers were then mounted on an optical translation stage with three axes of motion allowing for complete control over the focus of the optical excitation, which can be seen on the far left side of Figure 2.5A. A movable beamsplitter was used to image the illuminated area of the sample by focusing an image of the sample stage onto a charge coupled device (CCD) camera, as shown in Figures 2.4 and 2.5A. Using this technique, the beam diameter of the excitation was measured to be $d_m = 520 \pm 10\mu m$.

Figure 2.5: A. Photo of experimental photocurrent measurement setup as depicted by Figure 2.4. During experimental measurements the entire measurement apparatus was enclosed in a light-tight Faraday cage (not shown). B. Chip carrier containing wirebonded arrays of $N = 500, 200$ and $100$ SiNWs.


2.4 Results

2.4.1 Dark Current

The current-voltage (I-V) characteristics of arrays of $N = 500, 200$ and $100$ SiNWs are presented in Figure 2.6. All the I-V characteristics were measured at room temperature using a 150 W halogen light source focused through a microscope onto the SiNW arrays. The illuminated spot covered the full nanowire array, as well as the contact pads. It is important to note that in the region of zero bias, the measured dark current is four orders of magnitude lower than under illumination, demonstrating the low levels of noise present in the SiNW arrays and illustrating their suitability as photodiodes for light detection.

![Figure 2.6](image)

Figure 2.6: Current voltage characteristics of arrays of $N = 500, 200$ and $100$ SiNWs at room temperature, for bias voltages $-2 < V_{\text{bias}} < +2$ V.

One can see from Figure 2.6 it is theoretically possible to operate the SiNWs as avalanche photodiodes in order to improve device performance by utilizing avalanche multiplication, but it is not physically feasible. Consider the multiplication factor for a P-i-N diode [54].
\[ M = \frac{1}{1 - \int_{x_1}^{x_2} \alpha \, dx} \]  

(2.1)

Where \( \alpha \) is the carrier impact ionization coefficient, and \( x_2 - x_1 \) is the width of the intrinsic region of the diode in which avalanche multiplication may occur. Given that the intrinsic region in each individual SiNW is \( \approx 5 \times 10^{-5} \text{ cm} \), in order to achieve appreciable gain the diode must be biased such that the impact ionization coefficient is \( \alpha \approx 10^{5} \text{ cm}^{-1} \).

For both electrons and holes, this coefficient corresponds to an electric field value on the order of \( 10^{6} \text{ V/cm} \). As mentioned earlier, the SiNWs have an ultra-small cross sectional width of less than 10 nm, and applying fields of this magnitude could result in catastrophic failure in the nanowires. For this reason the SiNWs were not operated in an avalanche multiplication regime.

### 2.4.2 Responsivity

The power spectrum of the incident optical excitation was measured using a commercially available calibrated bulk silicon diode (Newport 818-UV) and is plotted in Figure 2.7. It is important to note that the difference in the characteristic shape of the spectra is due to a difference in halogen light sources and spectrometers used in the polarized and unpolarized measurements.

![Figure 2.7: Dependence of incident optical power \( P_m \) on wavelength for A. unpolarized, and B. arbitrarily polarized excitation.](image-url)
There is a large disparity between the illuminated area $A_m = \pi d_m^2/4$ and active area $A_a = NWL$ of the $N$ nanowire SiNW device, where each individual SiNW of width $W$ has a depletion region length of $L$. This disparity must be accounted for when calculating the responsivity of the active device $R$. First the raw responsivity, $R_{\text{raw}} = I/P_m$, was obtained for an unpolarized excitation. This quantity was then scaled by the difference between active and illuminated area according to $R = R_{\text{raw}} A_m/A_a$ and is plotted in Figure 2.8.

Figure 2.8: Measured dependence of responsivity $R$ on wavelength for $N=100$ (open triangles), 200 (open circles, offset 0.05 A/W), and 500 (open squares, offset 0.1 A/W), and theoretical fit.

Three distinct peaks at $\lambda \approx 420, 490-500$ and $540-560$ nm are evident in $R_{\text{raw}}$, for arrays of $N = 500, 200$ and 100 SiNWs. These resonances are not present in the well known absorption spectrum of bulk silicon [57], and are not trivial resonances of the air/SiO$_2$/Si cavity. Due to the small cross section of the individual nanowires, these resonances cannot be ascribed to a collective effect of leaky-mode resonances of the individual nanowires, which for $d \approx 10$ nm SiNWs in SiO$_2$ occur for $\lambda < 200$ nm [45,47].
Electronic quantum confinement effects in the optical absorption spectrum are also not a likely candidate for these resonances as the SiNWs do not have the necessary small diameter required to produce optical resonances, typically $d \approx 2\text{-}3\ \text{nm}$ \cite{58}.

As will be shown in Chapter 4, these observed resonances match predictions for the scattering of incident radiation into the SiNW grating. These resonances occur where radiation confined in the air/SiO$_2$/Si cavity accumulates phase from reflection at the interfaces and from scattering from the SiNW grating and interferes constructively. A metric to evaluate the ‘strength’ of these resonances is the resonance quality factor $Q$, which determines the lifetime of photons within the cavity. For each of the gratings the responsivity $R$ was fit to an exponential absorption background appropriate for bulk Si \cite{57}, modulated by resonances with a centre wavelength $\lambda_i$ and full-width half-max $\delta \lambda_i$. In Figure 2.8 the fits are plotted as solid lines alongside measured data.

### 2.4.3 Polarisation Response

The measured responsivity of the SiNW gratings retain the sinusoidal polarisation response expected from a single nanowire, primarily due to more efficient penetration of the electric field for parallel than perpendicular polarisation with respect to the nanowire axis \cite{59}. The measured dependence is shown in Figure 2.9 for the $N = 200$ SiNW grating, at a wavelength of 450 nm. The dependence of responsivity on polarisation can be written as $R = R_\parallel \cos(\theta) + R_\perp \sin(\theta)$ and this relationship is seen clearly in the sinusoidal fit in Figure 2.9. One can see that $R_\parallel > R_\perp$, which is the responsivity relation expected for semiconducting nanowires embedded in a dielectric structure (Figure 3.1). This reflects more efficient penetration of the electric field parallel to the nanowire axis, $E \parallel \hat{z}$, compared to the perpendicular orientation, $E \perp \hat{z}$. As discussed in the previous chapter, for a single SiNW embedded in SiO$_2$ we expect $R_\perp/R_\parallel \approx |2\varepsilon_{\text{SiO}_2}/(\varepsilon_{\text{Si}} + \varepsilon_{\text{SiO}_2})|^2 \approx 0.05$. The experimental value is much closer to 0.5 and falls short of the theoretical prediction.
Figure 2.9: Measured dependence of responsivity $\mathcal{R}$ on polarisation angle $\theta$ for $N = 200$ SiNW grating at $\lambda = 450$ nm. Error bars are associated with maximum fluctuations in current readout from the digital multimeter.

### 2.4.4 Gain

As mentioned earlier, when the number of charges collected in the measurement circuit becomes greater than one photogenerated pair per photon absorbed there is said to be gain. It is possible to estimate the gain in the SiNW gratings by comparing the measured value of responsivity to that of the theoretical value, which can be calculated from $\mathcal{R} = e\eta_{\text{int}} Q_{\text{abs}}/\hbar \omega$ (Equation 3.8) derived in Chapter 3, where there is gain $g = \eta_{\text{int}}$. The off-resonance zero-bias responsivity at $\lambda = 450$ nm is $\mathcal{R} = 0.075$ (Figure 2.9), which corresponds to $Q_{\text{abs}} = 0.020$ (Figure 4.4B), gives us a value of $g \approx 1$. This is in contrast with biased nanowire photoconductors, which frequently exhibit gain greater than 1000 \[6\]. This gain is most often attributed to fast trapping of either of the photogenerated electrons or holes at the surface, enhancing the lifetime $\tau$ of the complementary carrier. This allows the un-trapped carrier species to transit the device $g = \tau/\tau_{\text{tr}}$ times between contacts, where $\tau_{\text{tr}}$ is the carrier transit time. During this process, the ohmic contacts replenish the carrier of this species $g - 1$ times \[6\].

Closer examination of the band diagram in Figure 1.1 shows that replenishment of carriers is not possible near zero bias for a P-N junction nanowire. Electron (hole) replen-
ishment is strongly blocked by the P (N) region ohmic contact. Though electron (hole) replenishment is possible by the N (P) region’s ohmic contact, transport will be blocked by the junction’s built-in potential. This is interesting since gain from this process comes at the expense of bandwidth, and quenching the gain should increase intrinsic device speed \[32\]. It is possible to obtain gain by operating the P-N junction under reverse bias to enter the avalanche multiplication regime. Furthermore, a nanowire grating without P-N or P-i-N junctions could still exhibit resonances of $Q_{abs}$ in combination with photoconductive gain at finite bias. Any effect of inhomogenous electric field on the carrier mobilities would be absorbed into the device transit time $\tau_{tr}$, though such effects would be unlikely in the ultra-small nanowires employed here.
Chapter 3

Theory of Scattering and Absorption in Nanostructures

3.1 Definition of Responsivity

In order to validate and physically interpret the experimentally measured results of the previous chapter we must derive the relationship between absorption of the incident radiation in the SiNW grating and the resulting photocurrent spectra. As will be shown in the last chapter, this is also necessary to provide an avenue through which we may propose future devices to harness the selectivity and responsivity of a SiNW grating photodetector. All formulas and expressions presented in this chapter were derived from [60][61].

Consider a monochromatic plane wave incident normally on the SiNW grating of the form,

\[ \vec{E}_i(x, y, z, t) = \vec{E}_{i0} \exp(i(\omega t - \vec{k} \cdot \vec{r})) \]  

(3.1)

with wavevector \( \vec{k} \) and frequency \( \omega \). The dielectric structure will allow for photons of sufficient energy, greater than \( \hbar \omega \), to excite electron-hole pairs which will subsequently be swept to the contacts by the built-in field, generating current. Inside the dielectric
structure, the time-harmonic electric field may be written as

$$\vec{E}(x, y, z, t) = \vec{E}(x, y, z) \exp(i\omega t)$$  \hspace{1cm} (3.2)$$

which contains the incident and scattered electric fields. The net rate at which electromagnetic energy crosses a surface of area $A$ enclosing a volume $V$ is obtained by integrating the time-averaged poynting vector $\vec{S}$ over the surface,

$$W = -\int_A \vec{S} \cdot d\vec{A}$$  \hspace{1cm} (3.3)$$

where $d\vec{A}$ is the differential area with unit vector pointing outward, and $\vec{S}$ is the time-averaged poynting vector, which for a time harmonic field becomes, $\langle \vec{S} \rangle = 1/2 Re\{\vec{E} \times \vec{H}\}$. The negative sign in front of Equation (3.3) is merely convention for an outward facing unit normal. This implies that if the quantity $W$ is positive, there is a net transfer of energy into the volume (i.e. absorption). After algebraic manipulation we arrive at an expression for the amount of energy absorbed in the dielectric structure,

$$P_{\text{loss}} = \frac{1}{2} \int_V d^3r \epsilon_{im} \omega \left| \vec{E}(x, y, z) \right|^2$$  \hspace{1cm} (3.4)$$

where $\epsilon = \epsilon_r - i\epsilon_{im}$ and $V$ are the complex dielectric constant and volume of the dielectric structure, respectively. In this case, our dielectric structure consists of $N$ SiNWs of length $L$ and radius $R$, so we define the quantity $c_{\text{abs}}$ as,

$$c_{\text{abs}} = \frac{P_{\text{loss}}}{L|\vec{S}_i|} = \frac{\epsilon_{im} \omega}{\epsilon_0 c} \int_A d^2r \left| \frac{\vec{E}(x, y)}{\vec{E}_{i0}} \right|^2$$  \hspace{1cm} (3.5)$$

where $|\vec{S}_i| = \frac{1}{2} \left| \vec{E}_{i0} \right|^2 \epsilon_0 c$ is the time-averaged incident optical intensity of the monochro-
matic plane wave.

The photocurrent $I_{pc}$ generated in the semiconductor junction will be proportional to the number of electron-hole pairs generated by the power lost by the electric field to the junction. If we assume a fraction $f$ of the photo-generated pairs recombine in the junction, then the collected photocurrent is given by,

$$I_{pc} = \frac{e\eta}{\hbar\omega} P_{\text{loss}}$$

$$= \frac{1}{2} \frac{e\eta}{\hbar\omega} \epsilon_{im}\omega L \int_A d^2\vec{r} \left| \vec{E}(x,y) \right|^2$$

(3.6)

where $\eta = 1 - f$ and we have divided $P_{\text{loss}}$ by $L$ in order to change to a more convenient integral over the cross-sectional area of the SiNWs, as the electric field does not vary significantly in the axial direction. Responsivity $R$ is a measure of the electrical output per optical input and is defined as $R = I_{pc}/P_i$ where $P_i = 2RL|\vec{S}_i|$ is the incident optical power. Responsivity can then be recast in terms of our absorption cross section,

$$Q_{\text{abs}} = \frac{c_{\text{abs}}}{2R}$$

$$= \frac{\epsilon_{im} \omega}{\epsilon_0 c} \frac{1}{2R} \int_A d^2\vec{r} \left| \frac{\vec{E}(x,y)}{\vec{E}_{i0}} \right|^2$$

(3.7)

ultimately giving us,

$$R = \frac{e\eta}{\hbar\omega} Q_{\text{abs}}$$

$$= \frac{1}{2R \hbar\omega} \frac{\epsilon_{im} \omega}{\epsilon_0 c} \int_A d^2\vec{r} \left| \frac{\vec{E}(x,y)}{\vec{E}_{i0}} \right|^2$$

(3.8)
which is easily calculated in terms of well known variables, and the quantity \( \frac{|\vec{E}(x,y)|^2}{|\vec{E}_{in}|^2} \) which is the normalized square of the magnitude of the electric field within the nanostructure. This expression is easily obtained from finite element method (FEM) calculations of Maxwell’s equations described in the following chapter.

### 3.2 Polarisation Sensitive Phenomena

One of the more interesting phenomena related to semiconducting nanowires having a dielectric constant different from that of their environment is the emergence of polarisation sensitive effects. The optically-induced electric field that exists inside of a semiconducting nanowire is strongly dependent on polarisation and in turn has a prominent effect on various optical properties of the nanowires, including polarisation of luminescence, and modified optical absorption and photoconductivity when compared with their bulk counterparts [59].

Consider a cylindrical wire with dielectric constant \( \epsilon \) existing in an environment with dielectric constant \( \epsilon_{env} \) subject to an external electric field with parallel and perpendicular components, \( \vec{E}_0 = \vec{E}_{0\parallel} + \vec{E}_{0\perp} \). Maxwell’s equations state that at a dielectric interface the parallel component of the electric field must be continuous across the interface [44], giving us an identical value inside and outside the wire,

\[
E_{\parallel} = E_{0\parallel} \quad (3.9)
\]

Maxwell’s equations also state that across a dielectric interface the perpendicular component of the electric field will be discontinuous by an amount proportional to the surface charge induced on the surface [44]. This in turn leads to the perpendicular component of the electric field being suppressed,

\[
E_{\perp} = \frac{2\epsilon_{env}}{\epsilon + \epsilon_{env}} E_{0\perp} \quad (3.10)
\]
This equation holds for high frequency fields so long as the nanowire radius $R$ remains much less than the optical wavelength $\lambda$ [59]. This condition is easily met for the nanowires in this thesis, with $R < 10 \text{ nm}$ covering the entire infrared and visible light spectrum.

When the dielectric constant of the surrounding environment is greater than that of the nanowire ($\epsilon > \epsilon_{env}$) this implies two important consequences. First, when illuminating the nanowire with unpolarized light the induced component of the electric field parallel to the nanowire axis will be significantly larger and of high frequency. This will have a predominant effect on the polarisation of photons emitted during photoluminescence.

Secondly, and more importantly for the scope of this thesis, this means the amplitude of the induced electric field component parallel to the nanowire axis will be dramatically larger than the perpendicular component, significantly increasing the probability for optical transitions when the incident optical field is parallel to the nanowire axis. This implies that the ratio of parallel to perpendicular absorption coefficients will be,

$$\frac{k_{\parallel}}{k_{\perp}} = \frac{\epsilon + \epsilon_{env}}{2\epsilon_{env}} \epsilon_{env}$$ \hspace{1cm} (3.11)

In terms of the measurements performed in this thesis, the practical implication of this is that there will be significantly enhanced absorption, and hence photo-generated current, for incident optical excitation with polarisation parallel to the nanowire axis, and suppressed absorption for perpendicular polarisation. For an incident optical excitation arbitrarily polarized at some angle $\theta$ with respect to the nanowire axis (see inset of Figure 2.9), we can decompose the photocurrent response, and hence responsivity, of the nanostructure in terms of contributions from both parallel and perpendicular components as follows,

$$\mathcal{R} = \mathcal{R}_{\parallel} \cos \theta + \mathcal{R}_{\perp} \sin \theta$$ \hspace{1cm} (3.12)
Due to significantly suppressed responsivity for perpendicular polarisation, we expect the nanostructure to exhibit cosinusoidal dependence on polarisation angle $\theta$. Optical properties for Si in the visible wavelength range at $T = 300K$ were obtained from [58] in order to calculate the absorption ratio expected for silicon nanowires embedded in a SiO$_2$ environment with a dielectric constant of $\epsilon_{env} = 3.9$ [31] as shown in Figure 3.1.

It is important to note that the aforementioned polarisation sensitive phenomenon is derived purely from classical electrodynamics and does not consider the quantum mechanical nature of nanowires with large enough aspect ratio [59]. In extremely thin nanowires, when size quantization is present, the optical absorption matrix becomes anisotropic [62, 63], causing a deviation from Equation 3.11. In addition to designing polarisation sensitive photonic devices, this effect may also enable one to estimate the angular distribution of the orientation of ensembles of nanowires from their polarisation resolved absorption spectrum obtained by means of photoconductivity or photoluminescence measurements.

![Figure 3.1: Plot of responsivity ratio expected in Si nanowires embedded in SiO$_2$ for parallel to perpendicular polarisation of incident optical excitation.](image-url)
3.3 Resonance Quality Factor

The most appropriate metric one can use to compare the experimental and numerical results presented in this thesis, as well as relate the physical significance and understanding of the resonances to the photocurrent spectrum, is by means of the resonance quality factor $Q$. Physically, this factor represents the lifetime of photons within the cavity, and hence relates to the probability for absorption. For the experimental and numerical data presented in Chapters [2] and [4] respectively, $\mathcal{R} \propto Q_{\text{abs}}$ was fit to an exponential absorption background appropriate for bulk Si at energies relevant in the visible wavelength regime [57], modulated by individual gaussian peaks for each resonance. The mathematical form for a particular resonance takes the following form,

$$f(\lambda) = A_0 \exp \left( -\frac{(\lambda - C_0)^2}{2B_0^2} \right) + A_1 \exp \left( -\frac{\lambda}{B_1} \right)$$ \hspace{1cm} (3.13)

where $A_0, A_1, B_0, B_1$ and $C_0$ are free parameters fit to the experimental data.

Each peak has a centre wavelength of $\lambda$ and a full-width half-max of $\delta \lambda$. Thus, we define the quality factor as,

$$Q = \frac{\lambda}{\delta \lambda}$$ \hspace{1cm} (3.14)

In terms of the fitting parameters presented in Equation (3.13) the full-width half-max can be expressed as $\delta \lambda_i = 2\sqrt{\ln 2} B_0$ and the centre wavelength is simply $\lambda = C_0$. The overall $Q$ factor measured is an aggregate of various absorption and loss mechanisms $Q_i$ obeying,

$$Q = \left( \sum_i Q_i^{-1} \right)^{-1}$$ \hspace{1cm} (3.15)

As seen in Table [4.1] $Q$ is approximately independent of $N$ for the measured gratings ($N > 100$), so losses due to the finite number of SiNWs is not dominant.
Chapter 4

Numerical Results

4.1 Computational Methodology

Numerical simulations of the absorption efficiency $Q_{abs}$, and thus resulting Q factor, for various arrays of nanowires was performed using a Finite-Difference Time-Domain (FDTD) scheme \cite{64} implemented in the multiphysics commercial solver package COMSOL. COMSOL operates by discretizing the computational domain into a ‘mesh’ of elements and in turn solves Maxwell’s equations for each individual element of the domain, beginning with user-specified initial conditions, typically a magnetic or electric field distribution for the entire domain. Once COMSOL has solved the electric or magnetic field distribution for the domain of interest based on the initial conditions, it begins to leapfrog in time updating the magnetic field for the next time step based on the previous electric field, and then updating the subsequent electric field with the previous magnetic field and so on. Each field distribution for the subsequent time step is calculated based on the previous, complementary field distribution.
Chapter 4. Numerical Results

4.1.1 Model Geometry

The computational domain in the case of the encapsulated nanowire array structure presented in this thesis consists of periodic SiNWs embedded in a SiO$_2$ layer, enclosed by Si and air on either side, forming the optical cavity. As mentioned earlier, the nanowires are $L=1$ $\mu$m long and have a triangular cross sectional area with $w=6$ nm and $h=8$ nm. Due to the nanowire’s small cross sectional area in relation to the overall length of the nanowire, i.e. $d/L \ll 1$, the nanowires may be considered to be infinite and modeled as a two dimensional geometry. Furthermore, the nanowires were treated as $d=10$ nm cylinders and this assumption is validated in Appendix A where it is shown that the resonance wavelengths $\lambda_i$ do not depend on the specific cross-sectional geometry.

In this model we consider a cell of width $l=372$ nm, corresponding to the pitch or spacing of the nanowires. From top to bottom the computational domain is modeled as 600 nm of incident air, 400 nm of SiO$_2$, a $d=10$ nm cylindrical Si nanowire, 150 nm of SiO$_2$, and finally a 600 nm Si substrate. This can be seen in Figure 4.1.

![Figure 4.1: Schematic cross-section of Si nanowires embedded in SiO$_2$ supported by a Si substrate. The modeling domain is indicated by the shaded area.](image)

4.1.2 Material Considerations

The computational domain in the case of the nanowire array presented in this thesis consists of periodic SiNWs embedded in a planar dielectric cavity of SiO$_2$ enclosed by Si
and air on either side. In order for COMSOL to properly calculate the field strength and scattering behaviour in different media the complex dielectric permittivity, or equivalently complex refractive index, must be specified for each different material present for the domain of interest. In this case we are modeling the scattering behaviour of the array with respect to visible radiation, so the complex refractive indices \( n(\lambda) \) of Si and SiO\(_2\) must be specified for \( 400 \text{ nm} < \lambda < 700 \text{ nm} \).

### 4.1.3 Initial Conditions

In any FDTD simulation the two most important conditions necessary to produce physical results are arguably the source excitation and the boundary conditions for the system of interest. Without the appropriate source excitation, accurate results may not be extracted by means of misrepresenting the experimental measurements. This can potentially create non-physical artifacts in the simulation not present in the physical realization of the system. In addition, your source needs to be chosen properly such that your FDTD scheme is numerically stable and does not suffer from computational instabilities.

In addition to choosing the right mathematical form of source excitation (i.e. a plane wave source v.s. a Gaussian excitation), it is important to make sure the field is a physically accurate representation of the exciting field in the experimental measurements, taking into consideration reflections from the simulated structure. In order to properly realize a plane wave source that is a non-time decaying excitation one must implement the total field formulation.

Due to the linearity of Maxwell’s equations, the electric field may be decomposed into incident and reflected fields \([44]\),

\[
E_{\text{tot}} = E_{\text{inc}} + E_{\text{sc}}
\]  \hspace{1cm} (4.1)

Where \( E_{\text{inc}} \) is the electric field that would normally exist in the absence of scattering...
bodies, in this case nanowires, and represents the incident wavefront generated by a source, and $E_{sc}$ is the scattered field due to the structure.

In order to solve Maxwell’s equations in the presence of a scattering body, the incident field must be specified correctly for all regions of the structure. In this case this consists of the electromagnetic field in three regions: the air above the cavity, the SiO$_2$ film, and the Si substrate. One can numerically simulate these fields in COMSOL using an empty cavity absent of scattering bodies, and use the resulting field distribution as the excitation for the case of scattering. In the case of a planar structure such as the one described in this thesis, the field due to the cavity is easily calculated and may be specified analytically.

$$E_{inc} = \exp(ik_0(y - d_1))$$  \hspace{1cm} (4.2)\)

where $k_0$ is the free space wave-vector of the incident photon. The electric field is defined in this way such that at the air/SiO$_2$ interface, the magnitude of the field is unity.

![Diagram](image-url)
The Fresnel coefficients govern the amount of light that may be reflected or transmitted at an interface [60] and will determine the magnitude of the electric field in the film, due to multiply reflected light being trapped in the SiO$_2$ layer. The reflectivity coefficient is defined as the ratio of the reflected to incident electric fields at an interface and for polarisation parallel to the interface as is the case here, the reflectivities $r_1$ and $r_2$ at the SiO$_2$/air and SiO$_2$/Si interfaces respectively are defined as follows [60][61],

$$r_1 = \frac{n_{SiO_2} - n_{air}}{n_{SiO_2} + n_{air}}$$  \hspace{1cm} (4.3)

$$r_2 = \frac{n_{SiO_2} - n_{Si}}{n_{SiO_2} + n_{Si}}$$  \hspace{1cm} (4.4)

where $n_{SiO_2}$ and $n_{Si}$ are the real parts of the indices of refraction for SiO$_2$ and Si respectively. The magnitude of the reflected electric field at the air/SiO$_2$ interface is simply $E_R = E_{inc}(y = d_1)r_{inc}$ where $r_{inc}$ is the reflectivity at the air/SiO$_2$ surface and is equal to $-r_1$. Therefore, $E_R = -r_1$. This allows us to succinctly represent the electric field in air as,

$$E_{air}(y) = E_{inc}(y) + E_{ref}(y)$$  \hspace{1cm} (4.5)

$$= \exp(ik_0(y - d_1)) + E_R \exp(-ik_0(y - d_1))$$

Taking the transmission coefficient at the air/SiO$_2$ interface to be $t_1 = 1 - r_1$ we can calculate the amount of light transmitted at the air/SiO$_2$ interface to be,

$$E_t(y) = t_1 \exp(ik_f(y - d_1))$$  \hspace{1cm} (4.6)

where $k_f = k_0n_{SiO_2}$ is the wave-vector in SiO$_2$. After light passes through the air/SiO$_2$ interface it will begin its path through the SiO$_2$ film and undergo multiple reflections at each interface. Therefore, the electric field in the SiO$_2$ film will be a summation of all
Chapter 4. Numerical Results

fields after each subsequent reflection. This may be represented as,

\[ E_{\text{film}} = t_1 \exp(ik_f(y - d_1)) + t_1r_2 \exp(-ik_f(d_1 + d_2)) \exp(-ik_f(y + d_2)) \]
\[ + t_1r_1r_2 \exp(-2ik_f(d_1 + d_2)) \exp(ik_f(y - d_1)) \]
\[ + t_1r_1r_2^2 \exp(-i3k_f(d_1 + d_2)) \exp(-ik_f(y + d_2)) \]
\[ + t_1r_1r_2^3 \exp(-4ik_f(d_1 + d_2)) \exp(ik_f(y - d_1)) + \ldots \]
\[ = t_1 \exp(ik_f(y - d_1)) [1 + r_1r_2 \exp(-2ik_f(d_1 + d_2)) + (r_1r_2 \exp(-2ik_f(d_1 + d_2)))^2 + \ldots] \]
\[ + t_1r_2 \exp(-ik_f(d_1 + d_2)) \exp(-ik_f(y + d_2)) [1 + r_1r_2 \exp(-i2k_f(d_1 + d_2)) + \ldots] \]
\[ = t_1 \exp(ik_f(y - d_1)) \left[ 1 + \frac{r_1r_2 \exp(-2ik_f(d_1 + d_2))}{1 - r_1r_2 \exp(-2ik_f(d_1 + d_2))} \right] \]
\[ \text{(4.7)} \]

Using the well known Taylor series expansion of \((1 - x)^{-1} = 1 + x + x^2 + x^3 + \ldots\)
we can simplify Equation \(4.7\)

\[ E_{\text{film}} = \frac{t_1 \exp(ik_f(y - d_1)) \left[ 1 + r_2 \exp(-2ik_f(y + d_2)) \right]}{1 - r_1r_2 \exp(-2ik_f(d_1 + d_2))} \]
\[ \text{(4.8)} \]

Maxwell’s equations state that at a dielectric interface the electric field parallel to
the interface must be continuous across the boundary \[44\]. This allows us to recast the
electric fields in air and the Si substrate as,

\[ E_{\text{air}} = \exp(ik_0(y - d_1)) + (E_{\text{film}}(d_1) - 1) \exp(-ik_0(y - d_1)) \]
\[ E_{\text{Si}} = E_{\text{film}}(-d_2) \exp(k_\text{Si}(y + d_2)) \]
\[ \text{(4.9) (4.10)} \]

Using the final expressions derived in Equations \(4.8\) \(4.10\) allow one to properly specify
the incident electric fields for COMSOL that the SiNWs will be subject to.
4.1.4 Boundary Conditions

For the case of an infinite array of SiNWs, only one cell of the array is modeled in the computational domain, which allows for the boundary conditions to simply be set to periodic, shown in Figure 4.3A. For arrays with a finite number of SiNWs, an absorbing boundary condition is implemented to ensure scattered radiation is able to escape the computational domain. Without absorbing boundary conditions, the simulation is subject to spurious reflections from the boundaries which may produce non-physical results in the electric field and subsequent absorption cross section $Q_{abs}$ for the nanowire array.

Figure 4.3: SiNW grating cross-sectional unit cell as modelled in COMSOL for an A. infinite SiNW grating and a B. $N = 10$ SiNW grating, including mesh. All outer periphery boundary conditions are set to scattering boundary conditions, unless otherwise labeled.

Perfectly Matched Layers (PMLs) were implemented on the outer boundaries for the case of a finite system of SiNWs, shown in Figure 4.3B. PML is a lossy medium with a characteristic impedance matched to that of the adjacent computational domain, so as not to produce reflections from the computational domain/PML boundary [66]. Waves impinging on the PML are subsequently attenuated in each cell they traverse and can be absorbed for a wide range of incident angles. The outer boundary of the PML may be defined with either a scattering boundary condition, or as a perfect electric conductor, both of which produce the same result for the simulations undertaken in this thesis. The cross-sectional unit cell as modeled by COMSOL can be seen in Figure 4.3 including all said domains, as well as spatial meshing automatically generated by COMSOL.
4.2 Results

The first case considered is that of an infinite SiNW grating as discussed in the previous section and modeled exactly as shown in Figure 4.3A. Incident optical excitation with polarisation parallel and perpendicular to the nanowire axis is considered and the absorption cross-section $Q_{abs}$ is plotted as the solid and dashed trends respectively, shown in Figure 4.4A for $d = 10$ nm cylindrical nanowires. For parallel incident polarisation one can clearly see electric field enhancements at $\lambda = 423, 490$ and $544$ nm emerge in the SiNW grating, in good agreement with measurements. For perpendicular incident polarisation enhancements in the electric field are absent. This is essentially because the multiply scattered radiation by the array of SiNWs does not interfere constructively.

![Figure 4.4: A. Calculated cross sections for absorption $Q_{abs,\parallel}$ and $Q_{abs,\perp}$ for parallel and perpendicular electric field polarisations. B. Calculated cross sections for absorption in the visible wavelength regime for SiNW array in an air/SiO$_2$/Si cavity (solid line), an empty air/SiO$_2$/Si cavity ignoring scattering by SiNWs (dashed), and array of SiNWs suspended in SiO$_2$ ignoring scattering by the air/SiO$_2$/Si cavity (dash-dot).](image)

In order to further understand the absence of resonances for perpendicular polarisation, consider the excitation in the nanowires to be that of an induced dipole along the $\hat{x}$ axis. It is well known that dipoles do not radiate along their axis and as such the total field generated by all of the other nanowires at the location of the origin will be zero. The scattered field, which is multiply reflected by the interfaces may itself not be zero,
but is directed along $\hat{y}$, so our argument is still valid. This, combined with the fact that
the perpendicular component of the electric field intensity will be reduced by a factor of
$\left(\frac{2\epsilon_{env}}{\epsilon + \epsilon_{env}}\right)^2$ (≈ 20 at $\lambda = 400$ nm) as dictated by Equation 3.10, significantly suppresses the
resonances.

Additional calculations shown in Figure 4.4B give us further insight into the nature
of these resonances, and show that the SiNW grating embedded in the air/SiO$_2$/Si cavity
is responsible for the resonances, rather than the cavity itself. Scattering from a single
nanowire embedded in SiO$_2$ is too weak to exhibit strong resonant absorption, and the
empty cavity itself does not exhibit any enhancements in the electric field in the visible
wavelength regime, denoted by the dashed line. One can also see that an infinite SiNW
grating suspended in an SiO$_2$ medium without interfaces exhibits strong absorption at
only a single resonance in the visible wavelength regime, denoted by the dash-dot line.
This coincides with the onset of first-order Bragg diffraction satisfied by $l \sin \theta = \lambda_0/n_{SiO_2}$
for $\theta = \pi/2$. From these observations we can see that the interfaces of the air/SiO$_2$/Si
cavity modifies the resonance condition of the infinite SiNW grating to produce three
resonances in the visible spectrum.

Figure 4.5: A. Calculated absorption cross section $Q_{abs}$ for SiNW array gratings consisting
of N=10 (red), N=30 (green) and N=50 (blue) SiNWs. B. Calculated quality factors $Q$
for a finite and infinite number of SiNWs. The error associated with each Q-factor is a
root-mean-square deviation due to fitting of the numerical data.
The frequency of these resonances are in good agreement with the experimentally measured photocurrent response presented in Chapter 2 and are found to be within 5%. In order to further understand the behaviour of SiNW array gratings with a finite number of SiNWs additional calculations were performed for arrays of $10 < N < 100$ SiNWs as shown in Figure 4.5A. This allows us to determine the minimum number of nanowires necessary to observe enhancements in the absorption spectrum due to collective scattering effects, and to characterize the relationship between the sharpness of the peaks, and hence quality factors, and the number of nanowires in the grating. One can clearly see that the resonances may be reproduced for arrays consisting of as little as $N = 10$ SiNWs. Sharpening of the resonances, and thus improvement of $Q$, is predicted to occur rapidly as we approach $N = 50$ SiNWs and the overall $Q$ value reaches a practical maximum close to $N = 100$ wires, as can be seen in Figure 4.5B.

![Figure 4.6: Calculated scattered electric field distribution $|\vec{E}_{sc}|$ in the $\hat{z}$ direction shown for a single unit cell for $\lambda = 423, 490$ and 533 nm resonances.](image)

To gain a more intuitive understanding of these resonances it is helpful to consider the electric field profile of the SiNW grating system. In contrast to the leaky-mode resonances discussed in Chapter [1][15][47], enhancements exhibited by the SiNW grating are attributed to resonances in the electric field profile caused by collective effects of the SiNW array within the cavity, rather than the individual nanowires themselves as is the case for leaky-mode resonances. Depicted in Figure 4.6 is the scattered electric field profile $\vec{E}_{sc}$, for each of the resonances observed in the visible wavelength regime. One can
clearly see the standing wave pattern formed by the scattered electric field within the cavity, in which the SiNWs sit in close proximity to field maxima/minima, resulting in the enhancements observed in their absorption spectrum. For each particular resonance one can see the characteristic shape of the standing wave pattern. As we go to smaller wavelengths we observe a higher number of minima and maxima, corresponding to a higher mode number. It’s important to note that the field profile of the scattered electric field obtained for \( N = 10 \) SiNWs is identical to that of the infinite grating.

The experimentally measured and theoretically predicted free-space wavelengths \( \lambda_i \), full-width half-max \( \delta \lambda_i \) and Q-factors are presented in Tables 4.1 and 4.2 respectively.

<table>
<thead>
<tr>
<th>( N )</th>
<th>500</th>
<th>200</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda_1 ) (nm)</td>
<td>424 ± 1</td>
<td>419 ± 1</td>
<td>415 ± 2</td>
</tr>
<tr>
<td>( \delta \lambda_1 ) (nm)</td>
<td>37 ± 2</td>
<td>35 ± 1</td>
<td>32 ± 3</td>
</tr>
<tr>
<td>( Q_1 )</td>
<td>11 ± 1</td>
<td>12 ± 1</td>
<td>9.6 ± 1</td>
</tr>
<tr>
<td>( \lambda_2 ) (nm)</td>
<td>493 ± 1</td>
<td>510 ± 1</td>
<td>513 ± 3</td>
</tr>
<tr>
<td>( \delta \lambda_2 ) (nm)</td>
<td>29 ± 2</td>
<td>42 ± 2</td>
<td>26 ± 3</td>
</tr>
<tr>
<td>( Q_2 )</td>
<td>17 ± 1</td>
<td>12 ± 1</td>
<td>20 ± 3</td>
</tr>
<tr>
<td>( \lambda_3 ) (nm)</td>
<td>561 ± 2</td>
<td>546 ± 1</td>
<td>540 ± 5</td>
</tr>
<tr>
<td>( \delta \lambda_3 ) (nm)</td>
<td>55 ± 6</td>
<td>23 ± 3</td>
<td>43 ± 8</td>
</tr>
<tr>
<td>( Q_3 )</td>
<td>10 ± 1</td>
<td>24 ± 3</td>
<td>13 ± 2</td>
</tr>
</tbody>
</table>

Table 4.1: Experimentally measured free-space wavelengths \( \lambda_i \) and full-width half-max \( \delta \lambda_i \) and Q-factors for \( N = 500, 200 \) and 100 SiNWs.

<table>
<thead>
<tr>
<th>( N )</th>
<th>10</th>
<th>20</th>
<th>30</th>
<th>50</th>
<th>( \infty )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda_1 ) (nm)</td>
<td>422</td>
<td>423</td>
<td>423</td>
<td>423</td>
<td>423</td>
</tr>
<tr>
<td>( \delta \lambda_1 ) (nm)</td>
<td>10 ± 1</td>
<td>8 ± 1</td>
<td>8 ± 1</td>
<td>7 ± 1</td>
<td>6 ± 1</td>
</tr>
<tr>
<td>( Q_1 )</td>
<td>42 ± 2</td>
<td>52 ± 2</td>
<td>52 ± 2</td>
<td>60 ± 2</td>
<td>70 ± 3</td>
</tr>
<tr>
<td>( \lambda_2 ) (nm)</td>
<td>493</td>
<td>492</td>
<td>491</td>
<td>491</td>
<td>490</td>
</tr>
<tr>
<td>( \delta \lambda_2 ) (nm)</td>
<td>15 ± 1</td>
<td>12 ± 1</td>
<td>10 ± 1</td>
<td>8 ± 1</td>
<td>7 ± 1</td>
</tr>
<tr>
<td>( Q_2 )</td>
<td>32 ± 3</td>
<td>41 ± 3</td>
<td>49 ± 3</td>
<td>61 ± 3</td>
<td>70 ± 5</td>
</tr>
<tr>
<td>( \lambda_3 ) (nm)</td>
<td>553</td>
<td>549</td>
<td>546</td>
<td>546</td>
<td>544</td>
</tr>
<tr>
<td>( \delta \lambda_3 ) (nm)</td>
<td>20 ± 1</td>
<td>14 ± 1</td>
<td>10 ± 1</td>
<td>7 ± 1</td>
<td>5 ± 1</td>
</tr>
<tr>
<td>( Q_3 )</td>
<td>27 ± 3</td>
<td>39 ± 3</td>
<td>54 ± 4</td>
<td>78 ± 4</td>
<td>90 ± 20</td>
</tr>
</tbody>
</table>

Table 4.2: Theoretically predicted free-space wavelengths \( \lambda_i \) and full-width half-max \( \delta \lambda_i \) and Q-factors for \( N = 10, 20, 30, 50 \) and \( N \rightarrow \infty \).
Chapter 4. Numerical Results

The error associated with the Q-factor of each resonance is a root-mean-square deviation, and is due to fitting of the experimental and numerical data as described in Section 3.3.

4.3 Discussion

4.3.1 Reduction in Q-factor

Comparing the measured quality factors to that of the numerical results of an ideal, infinite grating, one can immediately see that the measured $Q$ for the $N = 500, 200$, and $100$ SiNW gratings appears to be independent of the number of nanowires in the grating. This is consistent with the trend observed in Figure 4.5B, but of significantly more importance experimentally is the fact that the measured quality factor ($Q \approx 10$) is approximately 7 times lower than the value of $Q$ predicted for the infinite grating. This indicates that there are considerable scattering losses incurred by the SiNW grating in this particular cavity, which I will attempt to explain and quantify in this section.

Simply put, since the decreased value of $Q$ means the lifetime of photons in the cavity is decreasing there are clearly loss mechanisms not considered in these numerical calculations. Photon absorption in the SiNWs (hence the resulting photocurrent), as well as in the Si substrate itself is accounted for in the model and is not responsible for the reduction in $Q$.

Another possibility is loss due to the finite size of the individual SiNW arrays, specifically loss of photons due to scattering at the boundaries of the cavity. Experimentally, this does not seem to be the case due to the relative constancy of the measured Q-factors with respect to $N$ (Table 4.1) for $N = 100, 200$ and $500$ SiNW arrays. If this were a dominant loss mechanism then it is to be expected that there should be a measurable increase in $Q$ as the number of SiNWs increases, which we do not find to be the case. Furthermore, referring to Table 4.2 one can see that the theoretical Q-factor is still approximately 5 times higher for as few as $N = 20$ SiNWs. In addition, the theoretical
upper limit for the Q-factor for \( N \to \infty \) is, for all intents and purposes, already achieved for \( N = 100 \) SiNWs, and loss of photons from the end facets is already accounted for in the finite \( N \) calculations with absorbing boundary conditions. For this reason we can reasonably assume the loss in \( Q \) cannot be attributed to the finiteness of the SiNW array.

Next let us assume that there is some sort of disorder introduced into the position of the individual SiNWs during the fabrication stage. Physically this could correspond to vibrations or deviations in the mask position during the lithography process described in Section 2.1, the effect of which is straightforward to calculate. Calculations of \( Q_{abs} \) were carried out for arrays of \( N = 100 \) SiNWs incorporating this disorder by adding a random deviation to the position of each individual SiNW. For root-mean-square deviations of up to 45 nm, \( Q_{abs} \) could not be reduced.

Having eliminated fabrication disorder and photon loss from the finiteness of the array, the most likely remaining explanation is due to the short (1 \( \mu m \)) length of the SiNWs, combined with their termination at conducting, ohmic contacts, which are not accounted for in the numerical calculations as the wires are assumed to be infinite in length. Significant scattering would occur at these conducting metal contacts compared to the mode of an infinite nanowire. By increasing the length of the SiNWs it should be possible to reduce scattering and absorption losses at the contacts, thus increasing the quality factor towards the theoretically predicted limit of an ideal, infinite array.

### 4.3.2 Device Design Improvements

Aside from eliminating the photon loss mechanisms described in the previous section, there are several possibilities to improve the opto-electrical performance of this SiNW grating based device. In this device, one of the main mechanisms for scattering losses is due to scattering of incident radiation into the Si substrate. We can coarsely evaluate this effect by replacing the Si substrate with vacuum, which forms a suspended film of SiO\(_2\) in which the SiNWs are embedded. Here, multiply scattered radiation by the nanowire
grating undergoes total internal reflection at each interface for radiation satisfying $\lambda > l$, rather than just at one interface. The resulting $Q_{\text{abs}}$ spectrum exhibits an enhancement of more than three orders of magnitude at each resonance in the visible wavelength regime as shown in Figure 4.7. One can clearly see how significant scattering losses incurred at the Si substrate are due to the observed sharpness of the resonances in Figure 4.7 when scattering losses are eliminated at the bottom of the SiO$_2$ interface.

![Figure 4.7: Calculated absorption cross section $Q_{\text{abs}}$ for fabricated structure (solid trend) and for SiNWs embedded in a suspended SiO$_2$ film with air interfaces on either side (dashed trend).](image)

By suspending this array in a similar manner, it should be theoretically possible to attain a quality factor over a magnitude higher than those measured here. This could be realized by selectively etching the underlying silicon on the supporting substrate, at least for a considerable portion of the total SiNW length. This would allow for photons in the air/SiO$_2$/air region of the cavity to experience total internal reflection and improve their lifetime in the cavity considerably. This, combined with a significant increase in the length of the SiNWs, could allow for a drastic increase in the quality factor of a SiNW grating based device.

Additionally, the electric field profile of the SiNW grating could be further optimized.
As can be seen in Figure 4.8, the SiNW is not spatially located directly at the maximum of the electric field profile. By designing an array in which each individual SiNW is located at a position of maximum electric field intensity, the probability for photon absorption could theoretically be increased proportionally to the square of the electric field, in accordance with Equation 3.6. It may also be worthwhile to explore the possibility of using asymmetric metallic end contacts, one schottky and one ohmic, in order to facilitate better carrier collection and further eliminate dark counts [67].

Figure 4.8: Calculated cross-sectional plot of normalized electric and magnetic field magnitudes for a single SiNW grating unit cell at the $\lambda = 544$ nm resonance. The SiNW position, 150 nm above the Si substrate, is denoted by a black circle.

4.3.3 Absorption Enhancement

We can further extend the results of this chapter to engineering ultrathin SiNW grating based devices which enhance sensitivity and selectivity of photodetection in the visible wavelength regime for a single wavelength. First, by simply reducing the thickness of the SiO$_2$ layer in which the SiNWs are encapsulated we can reduce the number of resonances to a single resonance. For the results presented, the SiO$_2$ thickness was reduced from 550 nm to 260 nm. By reducing the cavity size this has the effect of reducing the number
of trips photons may take in the cavity, and subsequently the length of time in the cavity \[41\]. This, combined with increased loss due to transmission at interfaces, means less resonances in the electric field are supported by the structure.

Next the grating period is altered in order to modify the resonance condition in such a way as to shift the wavelength of the supported resonance. Enhancements for red (\(\lambda \approx 610\) nm), green (\(\lambda \approx 540\) nm), and blue (\(\lambda \approx 460\) nm) wavelengths are obtained for grating periods of \(l_R = 460\) nm, \(l_G = 400\) nm, and \(l_B = 320\) nm, respectively. The enhancement in the electric field can be seen in Figure 4.9 for \(d = 20\) nm SiNWs. In terms of fabrication, these adjustments are straightforward and merely require a different mask and shorter dry oxidation times than those mentioned in Chapter 1.

Figure 4.9: Electric field enhancement factor inside \(R=10\) nm SiNWs embedded in 260 nm thick SiO\(_2\) for red, green and blue wavelengths with grating periods of \(l = 460, 400,\) and \(320\) nm respectively.

The immediate application of designing these ultrathin SiNW grating devices with increased sensitivity and selectivity is the detection of white light. In principle, white light detection or the detection of visible radiation may be achieved using linear detectors with spectral responsivities similar to that of the cones in the human eye \[68,69\]. This concept of colour perception is a well understood field and was first scientifically defined
by the International Commission on Illumination (CIE) as CIE 1931 colour space, based on a series of experiments performed by William David Wright and John Guild in the late 1920s. The results of these experiments allowed Wright and Guild to map all of the colours of the visible spectrum (detectable by the human eye) into the CIE XYZ colour space, a mathematical model which in principle can describe any colour.

Though still a subject of much debate, the photoreceptor cones in the human eye have been found to have spectral sensitivities that peak at short (≈ 420 nm), medium (≈ 530 nm) and long (≈ 560 nm) wavelengths. In the experiments performed by Wright and Guild, the normalized spectral responsivities of the human eye were mapped in terms of tristimulus values. These values correspond to amounts of primary colours that may be used in an additive model to effectively simulate any visible colour. Due to the fact that colour detection depends heavily on the observers field of view, three colour mapping functions (cmf) were defined in this model to describe the chromatic response of a standard observer. The tristimulus values are given as follows,

\[
X = \int_{380}^{780} I(\lambda) \bar{x}(\lambda) d\lambda \\
Y = \int_{380}^{780} I(\lambda) \bar{y}(\lambda) d\lambda \\
Z = \int_{380}^{780} I(\lambda) \bar{z}(\lambda) d\lambda
\]

where \( \lambda \) is the wavelength, \( I(\lambda) \) is the spectral power distribution and \( \bar{x} \), \( \bar{y} \) and \( \bar{z} \) are the cmfs.

By designing linear photodetectors that recreate these colour mapping functions or responsivities, as shown in Figure 4.10, it is possible to design a platform to detect visible radiation similar to the mechanism used by the human eye. The immediate advantage of using ultra-thin SiNWs for such a device becomes apparent when we consider the current size of pixels in current digital imaging technologies. In current digital camera technology
the average pixel size is on the order of 50-100 $\mu m^2$ [74]. By creating devices with the SiNW gratings presented in Figure 4.9 with a modest number of NWs ($\approx 20 - 30$) we can nearly halve current pixel size, while achieving substantial responsivity and reduced dark counts due to the low volume of the SiNWs. Furthermore, due to the anisotropic polarisation response observed in these arrays combined with the increased sensitivity over bulk devices, it is very possible to ‘stack’ these pixels in an orthogonal orientation to further reduce pixel size while avoiding saturation of individual pixels.
Chapter 5

Summary

5.1 Conclusions

In this thesis, the optoelectronic properties of an ultrathin Si nanowire resonant grating nanostructure is examined in detail, experimentally by spectral photocurrent spectroscopy, and numerically by finite-difference time-domain calculations. The measured visible wavelength resonances are found to be in excellent agreement with the mechanism of antenna enhancement due to scattering of incident radiation into geometrical resonances supported by the SiNW grating.

A quality factor of \( Q \approx 10 \) was measured for gratings consisting of \( N = 500, 200 \) and 100 SiNWs for the \( \lambda = 420 \) nm resonance. Theoretical calculations for arrays of infinite length SiNWs give a quality factor of \( Q = 70 \pm 10 \), noticeably higher than that of the experimentally measured results. The reduction in \( Q \) factor is attributed to additional photon loss originating from the short length of the finite SiNWs (1 \( \mu \)m) and their termination at conducting, ohmic contacts. This may be improved upon by considerably increasing the length of the SiNWs and reducing scattering by the contacts. For infinite length SiNWs, incomplete reflection occurs at the SiO\(_2\)/Si interface, which is the dominant loss of radiation from the cavity. Numerical calculations show that by
suspending the SiO$_2$ encapsulated nanowires the $Q$ factor can be increased by several orders of magnitude.

Sinusoidal polarisation anisotropy expected from single nanowires was observed in the SiNW array for linearly polarized radiation, with the strongest response for $\mathbf{E} \parallel \hat{z}$ (i.e. parallel to the nanowire axis), while for $\mathbf{E} \perp \hat{z}$ the resonances are suppressed. This reflects more efficient penetration of the resonant field into the SiNW for $\mathbf{E} \parallel \hat{z}$ case and is consistent with numerical calculations.

Finally, it is shown that field enhancement is easily engineered into SiNW gratings by a thoughtful choice of SiO$_2$ thickness and grating period. First, by reducing the thickness of the encapsulating SiO$_2$ layer the number of resonances in the visible wavelength regime is reduced to one. Second, by carefully choosing the grating period the individual resonance supported by the SiNW grating may be blue or redshifted to the desired frequency. This, combined with the polarisation dependent response, allows for the potential of designing a visible wavelength colour photodetector in which pixels may be further reduced in dimension by orthogonalizing the SiNW gratings.

These observations provide a framework for engineered, grating based enhancement of the light-matter interaction in one-dimensional nanowire structures and the design of nanowire antenna-enhanced photodetectors, with enhanced wavelength and polarisation sensitivity. Furthermore, these results extend the theory and application of single nanowire optical resonances in photoconductors to the limit of collective scattering in large arrays. Further work is necessary to fully understand the antenna effects in arrays of larger diameter nanowires outside the Rayleigh scattering regime, and examine the possibility of more complicated, resonant structures.
5.2 Future Perspectives

It is obvious that there are not only a variety of physical mechanisms through which the detection of radiation is possible, but there are a great many ways to construct and enhance said devices to tailor them to specific purposes, say for the high speed detection of visible radiation, or low level light detection of infrared radiation as an example. Given the current state of photonics, and in particular solar energy generation and optical communication, it is no surprise that detection of a wide range of radiation from the ultraviolet to infrared is of paramount importance to continue realizing the most efficient and cutting edge manifestations of these technologies.

The resonantly balanced, detection platform presented in this thesis is well suited to the detection of moderate intensity visible radiation for kHz operation. The responsivity of this detector was characterized using the technique of photocurrent spectroscopy, which is a far-field optical technique, giving information on the overall magnitude of the electric field inside the SiNW structure. This technique is non-invasive and is adept at determining the responsivity, but gives no information about the near-field optical or electronic properties of the structure.

This thesis presents experimental and numerical results for a very simple paradigm for optical sensing, demonstrating basic techniques for designing and characterizing a photodetector. In order further advance the technologies mentioned earlier, increased sensitivity down to single photon levels and reduced response time need to be engineered into nanowire photodetectors.

Though silicon is an attractive material due to its well understood physical properties, availability and ease of integration with current SOI thin film technologies, its indirect bandgap not only reduces the amount of absorption possible, but requires phonon generation to conserve momentum, generating more noise. Direct bandgap materials such as InAs are an attractive alternative to this, combined with the ease in growing lattice mis-matched structures on various substrates, means they are growing increasingly more
suitable for integration with current and future nanoelectronic devices \[75, 76\] and provide a platform for detecting visible and infrared radiation \[76, 77\]. Furthermore, carriers in InAs have lower effective masses, thus facilitating faster collection of carriers \[78\].

More robust, non-invasive, scanning probe techniques should be implemented to study these nanowire structures to gain additional details into the physical properties that make them suitable for photodetection. One example of this is scanning gate microscopy \[79\], in which the electrical and carrier transport properties may be probed on a local scale by introducing a small electrostatic perturbation close to the surface of the nanowire by means of a conducting tip of an atomic force microscope (AFM). This technique can provide spatial information on the order of the \(\lambda_F/2\), where \(\lambda_F\) is the Fermi wavelength \[79\].

Another such technique is near-field scanning optical microscopy (NSOM), in which local illumination of the photodetector reveals spatial variation and bias dependence, which in turn determine photocarrier transport and collection properties \[80, 81\]. By placing the detector much closer to the surface in NSOM, one can probe the evanescent fields which only exist very near to the surface. Additionally, because the detector is so close to the surface, more of the diffracted light may be collected, allowing for resolution greater than the Rayleigh criterion.

By combining the experimental methods and techniques presented in this thesis and exploring InAs nanowire based photodetectors, characterizing them using the more advanced, but non-invasive scanning probe techniques mentioned, it is possible to engineer much more efficient and responsive photodetectors used in the detection of radiation from the visible, into the infrared.
Bibliography


Appendix A

Nanowire Geometry

In order to validate the choice of cylindrical $d = 10$ nm cross-section nanowires in the numerical calculations, a variety of geometries were modeled for comparison. As discussed in the main text, the triangular SiNWs were considered to be independent Rayleigh scattering bodies, meaning the calculated absorption efficiencies and resonant line widths should be relatively independent of the individual nanowire geometries and diameters. From Figure A.1 it is confirmed that the line width of a triangular nanowire with cross-sectional area 78 nm$^2$ closely matches that of the $d = 10$ nm cylindrical nanowire with area 78.5 nm$^2$. This shows that the Rayleigh regime well describes the nanowire grating for $d/\lambda \approx 1/30$. 
Figure A.1: Comparison of calculated absorption efficiencies for cylindrical SiNWs of diameters $d = 10$, 8, and 6 nm and triangular cross section SiNWs with $w = 13$ nm and $h = 12$ nm.
Appendix B

Contributions