

**Dimensional Dependence of Light Interaction with Nanowires**

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by

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of

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## DEDICATIONS

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This thesis is dedicated to my family. Their unconditional support and love was the foundation of success for my graduate study. I want you to know that I love you so much and this thesis was only possible thanks to you.

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## ABSTRACT

Dimensional Dependence of Light Interaction with Nanowires

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Advisor: Dr. Bahram Nabet

Semiconductor nanowires have been used in a variety of passive and active optoelectronic devices including waveguides, photodetectors, solar cells, LEDs, Lasers, sensors, and optical antennas. We have designed and fabricated GaAs/AlGaAs core-shell nanowires (CSNWs) grown on both GaAs and Si substrates by vapor-liquid-solid (VLS) method. These nanowires show extremely enhanced optical properties in terms of absorption, guiding, radiation of light, and even lasing. Analysis of the interaction of light with cylindrical and hexagonal structures with sub-wavelength diameters identifies both transverse plane modes and longitudinal plane modes in a generalized volumetric resonance modes without the need for vertical structures such as Bragg mirrors commonly used in vertical cavity surface emitting lasers (VCSEL's). We report on FDTD simulations with the aim of identifying the dependence of these modes on: geometry (length, width), tapering, shape (cylindrical, hexagonal), core-shell versus core-only, and dielectric cores with semiconductor shells. This demonstrates how NWs form excellent optical cavities without the need for top and bottom mirrors. However, optically equivalent structures such as hexagonal and cylindrical wires can have very different optoelectronic properties meaning that light management alone does not sufficiently describe the observed enhancement in upward (absorption) and downward transitions (emission) of light in nanowires; rather, the electronic transition rates should be considered. We discuss how the transition rates change with respect to electron distribution and identify three factors explicitly contributed to the transition rates with strong dependence on dimensionality. In addition, a CSNW based laser has been proposed and modeled, showing large increase in optical gain and quantum efficiency compared to their bulk counterparts. These results and findings will further facilitate the design and optimization of sub-micron scale optoelectronic devices. In conclusion, we make a case for photonic integrated circuits that can take advantage of the confluence of the desirable optical and electronic properties of these nanostructures.



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## CHAPTER 1

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### INTRODUCTION

The practice of staining glass for decorative purposes dates to ancient Rome, but the investigation of light matter interaction starts even back to the beginning of history for human beings, when ancient peoples first notice the existence of sun or the first time to use torch for hunting. People never stop to study how the light interact with our world, meanwhile, implement our understanding to build a better world with lighting technology. The stained-glass windows such as the one inside of the St. Patrick's Cathedral in Fig. 1.1 served as a 'poor man's Bible' in the Middle Ages, allowing believers who could not read Latin to learn the story of the Gospels. The term stained glass refers to glass that has been coloured by adding metallic salts during its manufacture. Then this coloured glass is crafted into stained glass windows in which small pieces of glass are arranged to form patterns or pictures. Even nowadays, people are still surprised about how beautiful they are and wondering how the light interact with these pieces of art crafts. Besides the arts, lighting technology is also evolving very rapidly, from the ancient torches to the bulb that Thomas Edison invented and to the modern LEDs such as the one in Fig. 1.1. From blackbody radiation to electroluminescence, i.e., from thermal radiation to electrons-holes recombination, we are now capable to generate light more clean and more efficiently.

Now we find ourselves living through a new revolution in the age of information technology, one with consequences every bit as dramatic and likely even more profound as the data transmission by light. Electrons served us very well for the recent few decades, until the explosion of data growth nowadays. The storage and the transmission of data consumed large amount of power and

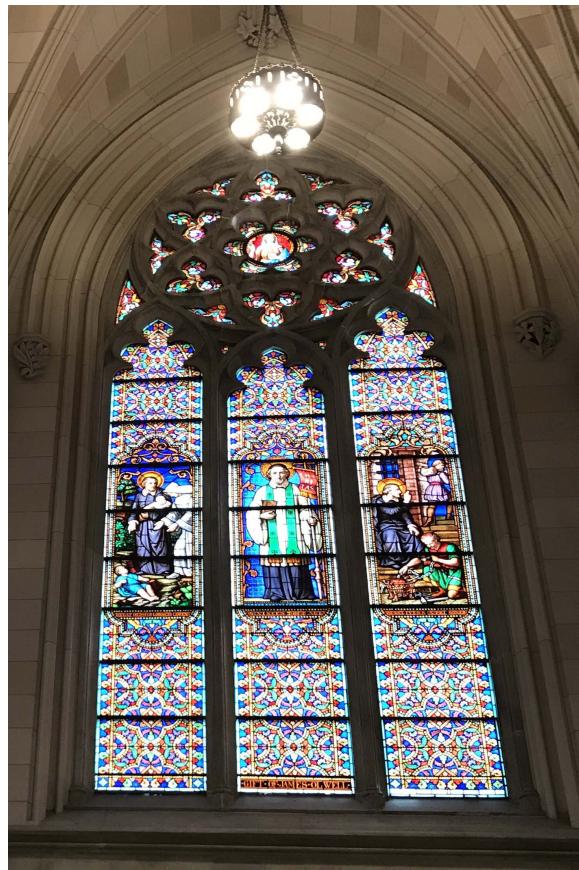


Figure 1.1 The Stained-glass window and the top modern lamps inside of the St. Patrick's Cathedral, 5th Ave, New York, NY.

time, simultaneously. Meeting the energy needs of the communication of information, together with storage and computation form a "grand challenge" of the information age.

One good example of huge amount of power consumption by data transmission and computation is the data centers, which currently consume 1.5% of global energy production, and up to approximately 4% of U.S. energy produced. Though the statistics seems small, a 1000 times increase in the volume of data is predicted by 2025. Google data center alone consumes enough electricity to power 200,000 homes, since an average Google search or a YouTube video or a message through Gmail uses 0.3 watt-hours of electricity. Having efficient data computation and transmission tools will greatly reduce the total data center power consumption into a greener number. And the data pipelines of light can certainly be very helpful in this regime.

## 1.1 Background

### 1.1.1 Photonics and Optoelectronics

Photonics involves the generation, control and detection of light waves and photons, which are particles of light, in free space or in matter. Optoelectronics is the study and application of effects related to the interaction of light and electronic signals, and usually considered a sub-field of photonics. Both photonics and optoelectronics study the light, and explore a wider variety of wavelengths besides visible lightwave range, from gamma rays to radio, including X-rays, ultraviolet and infrared light.

The invention and development of solar cells<sup>3,4</sup>, photodetector<sup>5,6</sup>, modulators<sup>7,8</sup>, LEDs<sup>9–11</sup> and lasers<sup>12,13</sup> certainly set the example of breakthroughs due to the manipulation of photons in thin films and semiconductor bulk crystals. The continuing success of photonic technologies relies on the discovery of new optical materials and the miniaturization of optoelectronic devices that feature better performance, low cost and low power consumption. For the last few decades, countless efforts in nano-scale materials and devices research has created a rich collection of nanostructures where size, shape and composition can be readily controlled. Many such nanostructures exhibit fascinating optical properties that could have significant impact in the future for photonic technology.

### 1.1.2 Core-Shell Nanowires

The primary principle for constantly miniaturizing the device is not only about the size, but also to have better electronic and optical properties. And this is achieved by quantization, or to be more specific, the confinement of electrons and photons. At the very dawn of electronics, the idea of using heterostructures (i.e., the structure with two layers or regions of dissimilar crystalline semiconductors) has emerged. After Shockley proposed the idea, Alferov and Kroemer introduced the concept that heterojunctions could possess high injection efficiencies in comparison with homojunctions, and we know now which is due to the confinement of carriers<sup>14</sup>. It would be very difficult today to imagine solid-state physics without semiconductor heterostructures for both electronic-based and optical-based applications. The heterostructures and especially double heterostructures, including quantum wells, nanowires, and quantum dots, are the fundamental building blocks for current nanoscience research as depicted in Fig. 1.2.

Quantum well is a potential well which confines particles to only move freely in two dimensions instead of three dimensions, by forcing them to occupy a planar region. These wells are formed in semiconductors by having a narrower bandgap material sandwiched between two layers with wider bandgap materials. Electrons in quantum wells are confined in two dimensions either naturally or by doping the barrier of a quantum well, thus a two-dimensional electron gas (2DEG) may be formed at the heterointerface. Not only an increasing of the density of states, but also a better performance in optoelectronics devices such as laser diodes, High Electron Mobility Transistors (HEMTs), photodetectors, and solar cells.

Quantum dots, as another most common nanostructure in semiconductor physics, exhibit much more enhanced optical properties. They are normally only several nano-meters in size, and either synthesized or self-assembled into a bulk solid. As the particles in the quantum dots are confined in three dimensions, which leave them zero degree of freedom. As a result, the density of states changed to a delta function compare to a smooth square root dependence that is found in bulk materials. The narrower peak spectra and larger magnitude of intensity make them even better candidates in

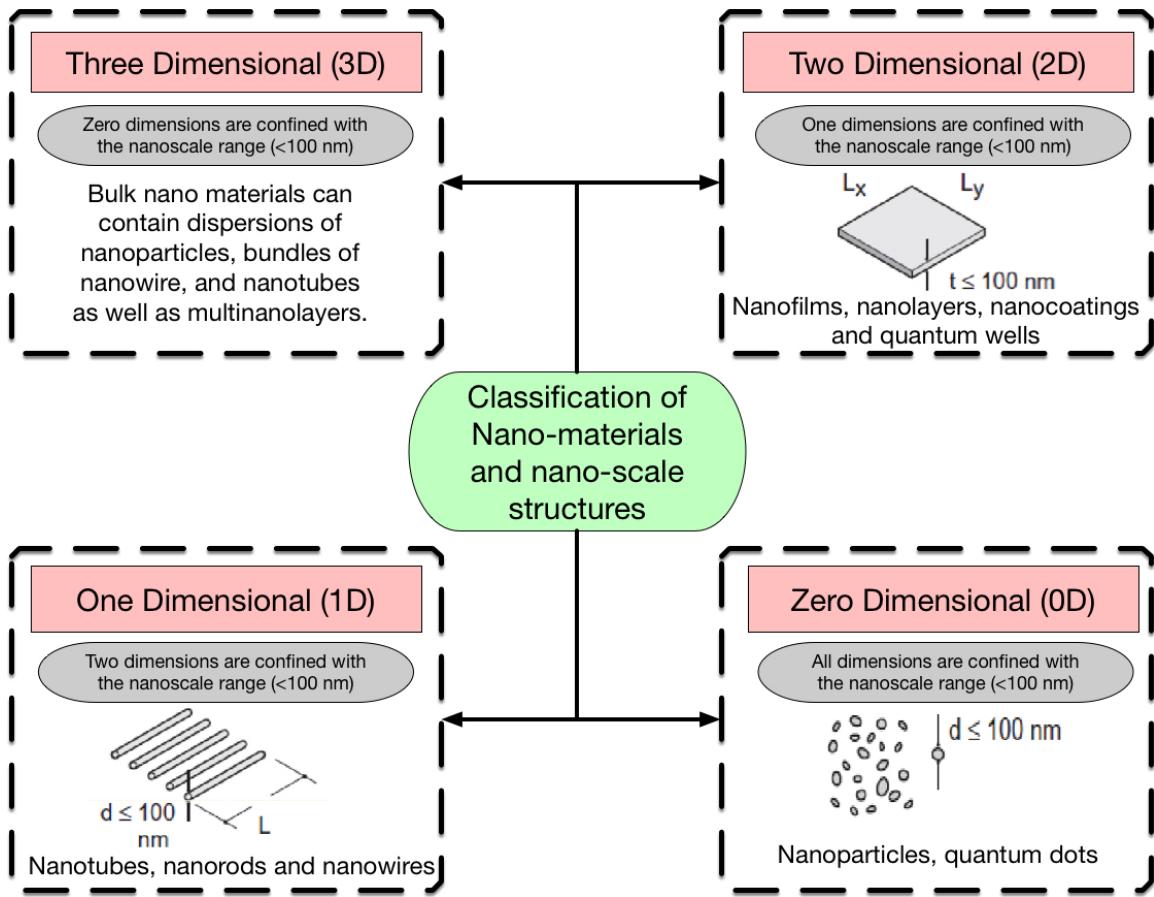


Figure 1.2 Diagram of classification of nano-materials and nano-scale structures

the application of solar cells, lasers and light emitting diodes (LEDs).

However, since the introduction in the 1990s, another important class of semiconductor nanostructures has emerged: structures with cross-sections of tens or hundreds of nano-meters and lengths up to several micro-meters. These structures are named as 'nanowires'<sup>15</sup> different from quantum dots as they are confined only in two dimensions, thus allowing electrons, holes or photons to propagate freely along the third dimension. Besides their own outstanding electro-optical properties, the high-aspect-ratio of these new semiconductor nanostructures allows for the bridging of the nanoscopic and macroscopic world. As Dr. Peidong Yang said in their review paper, "This nano-macro interface is fundamental to the integration of nanoscale building blocks in electrical or optoelectronic device applications. Conventional photonic platforms often consist of features with large aspect-ratios such as interconnects and waveguides, typically with micrometre dimensions. Thus, when semiconductor nanowires emerged they were immediately recognized as one of the essential building blocks for nanophotonics."<sup>16</sup>

The development of sophisticated nanowires growth techniques<sup>17,18</sup>, either bottom-up<sup>19,20</sup> or top-down<sup>21</sup>, has stimulated a large body of new work in semiconductor nanowires over the last twenty years or so. Previously, the research activities focus on the growth of higher quality nanowires<sup>22</sup> and the variation of materials. At that time, most of the nanowires are core-only with ZnO<sup>22</sup>, GaAs<sup>23</sup>, Si<sup>24</sup>, or Ge<sup>25</sup>. However, later on, researchers found out that growing an additional layer of shell can increase quantum yield by passivating the surface trap states. In addition, the shell provides protection against environmental changes, photo-oxidative degradation, and provides another route for modularity. Precise control of the size, shape and composition of both the core and the shell enable engineering the device with many degree of freedom and optoelectronic properties, such as the emission wavelength is able to be tuned over a wider range of wavelengths than with either individual semiconductor. Undoubtedly, much of this interest was further stimulated by the possibility of novel physics and applications in core-shell nanowires.

The successes of semiconductor nanowire optoelectronics and promising physical mechanisms using

quantum-confined structures have, furthermore, enlivened the debate over possible applications of optics for functions such as transmission, logic and switching in communications and computation. It is important to emphasize at the outset that quantum confinement and produce not only quantitative but also qualitative differences in physics from that in bulk structures, which is of course another major motivation for the interest in them. As Dr. Miller discussed in the paper about quantum well:<sup>26</sup> "There are many examples of these differences. The optical absorption spectrum breaks up into a series of steps associated with the quantum-confined electron and hole levels. Excitonic effects become much stronger because of the quantum confinement, giving clear absorption resonances even at room temperature. The relative importance of direct Coulomb screening and exchange effects is quite different in quantum wells (the Coulomb screening is relatively much weaker), giving very different optical saturation behaviour." Similar to quantum well, but nanowires have been observed even more profound differences in physics. Thus, the analysis and discussion about different behaviour of nanowires and bulk semiconductors when they interact with light will be the primary topic of this dissertation.

## 1.2 Literature Review

Since the introduction of initially so-called 'nanowhiskers' in the 1990s<sup>27</sup>, semiconductor nanowires have been extensively studied and much insight has been gained on tuning their electrical and optical properties. Nanowire related articles have shown a healthy increase in number published from 2005 to 2016, as Fig. 1.3 (blue bars) shows. Article with topics on optical properties of nanowires comprise a good portion in all the nanowire-related papers published in the recent decade, showing clear increasing trend in the number of papers on NW optics or photonics (green bars), presently comprising more than four-fifth of the nanowire-related articles.

The applications and classifications of NWs are shown in Fig. 1.4. In terms of the geometric structure, the most common NWs are cylindrical<sup>28,29</sup> and hexagonal<sup>30,31</sup> due to the growth techniques. And as discussed previously, there are core-only<sup>32-34</sup>, core-shell<sup>35,36</sup> and core-multi-shell<sup>37,38</sup> configurations in order to exploit various properties of NWs. In addition, NWs have been used as electronic

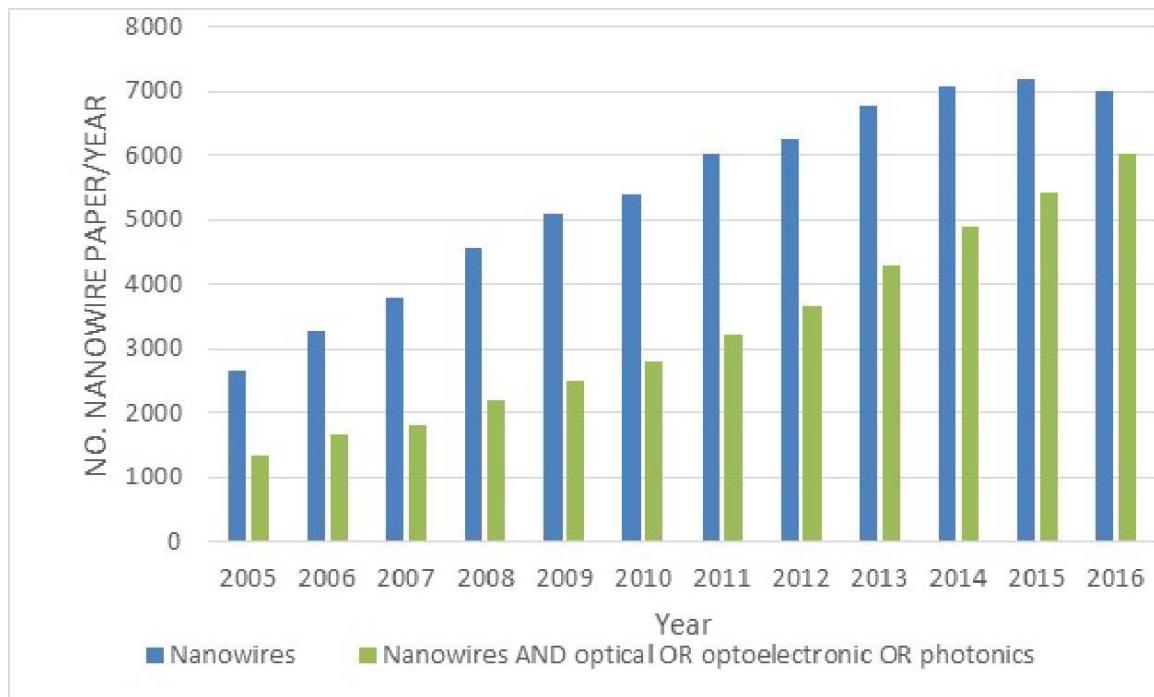


Figure 1.3 Article with topics on optical properties of nanowires consist of a large portion of all the nanowire realted papers published from 2005 to 2016. (Source: ISI website, keyword: Nanowire (blue), Nanowire AND optical OR optoelectronic OR photonics (grey))

based devices, such as High Electron Movement Transistors (HEMTs)<sup>39,40</sup>, Field Effect Transistors (FETs)<sup>41–43</sup>, capacitors<sup>44</sup>, diodes<sup>45,46</sup>, and optoelectronic based devices, such as lasers<sup>2,34,47–53</sup>, LEDs<sup>54–58</sup>, Solar Cells<sup>59–65</sup>, Photodetectors<sup>28,66–70</sup>, waveguides<sup>71–75</sup>, phototransistors<sup>76–80</sup>.

Exciting developments have been made in the academia environment from many research groups worldwide, including notably the Lieber group at Harvard University<sup>34,39,52,53,81,82</sup>, the Yang group at Berkeley<sup>18,22,69,83,84</sup>, the Samuelson group at Lund University<sup>45,68,85–87</sup>, and the Wang group at Georgia Tech<sup>33,88–92</sup>. With different angles, these research groups focus on a variation of NW materials, growth techniques and applications as shown in Fig. 1.4. The development of semiconductor NW materials follow the similar road as bulk materials, from initial single element (e.g., Si<sup>24</sup>, Ge<sup>25</sup>, Carbon<sup>93</sup> et al.) to compound binary (ZnO<sup>83</sup>, GaN<sup>53,94</sup>, CdSe<sup>78</sup>, ZnS<sup>95</sup>, ZnSe<sup>96</sup>, InP<sup>80</sup>, CdS<sup>95</sup>, GaAs<sup>97</sup> et al.), ternary (InGaAs<sup>98</sup>, CdSSe<sup>99</sup>, AlGaN<sup>100</sup>) or even quaternary (AlInGaN<sup>101</sup>), then to currently popular III-V heterostructure NWs(e.g., GaAs/AlGaAs<sup>102,103</sup>, GaAs/InGaAs<sup>104</sup>,



Figure 1.4 Diagram of nanowires applications and classifications

InGaN/GaN<sup>105</sup>, GaAs/GaAsP<sup>51</sup> et al.). At the same time, many important electronic and optical properties have been observed, and some of the fundamental applications have been demonstrated as well. The first optical pumped nanowire laser was demonstrated by the Yang group<sup>20</sup> at 2001, and two years later, the Lieber group shown the first electrical injected nanowire laser<sup>34</sup> which makes NW a potential candidate to be integrated in the electronic based integrated circuits.

In the field of industry and commercialization, some companies have started their adventure in the areas like energy, environment, biomedical et al., with their products that influencing our daily life. The glo-USA, Inc.<sup>106</sup> is a LEDs manufacturing company at Sunnyvale, CA. They use nanowire arrays which fabricated on chip to generate light as shown in Fig. 1.5(a). Each nanowire acts basically as an individual light-emitting diode (LED) with two circular metal contacts as anode and cathod. The inset is the 45 degree magnified view of the NW array. Except the fabricated blue nLED as in Fig. 1.5(b), all color of the visible spectrum, ranging from deep blue to red, can be realized using nanowire LEDs with industry-standard semiconductor material and manufacturing equipment. Since these nanowires are made using one material system with the active layers grown on the non-polar plane, they can reduce the wavelength shift and efficiency drop that are observed with other commercially-available planar LEDs. This will enable a true white RGB (red, green and blue) LED without the need of lossy phosphor conversion, thus achieving the highest Color Rendering Index (CRI) and efficiency.

From academic research to industrial applications, from efficiently electrons transportation to high quality light confinement, and from applications for environment concern to electronic devices in the daily life, the interaction of light and nanowires need to be investigated, thus, the major topic of this dissertation is to study the optoelectronics properties of core-shell nanowires and how they interact with light when electrons in this nano-scale structure are confined in lower dimensionality.

### 1.3 Scope and Organization of the Dissertation

This thesis is structured as follows. The growth techniques and electro-optical properties of core-shell nanowires are presented in Chapter 2. After introducing four different light confinement mechanisms,

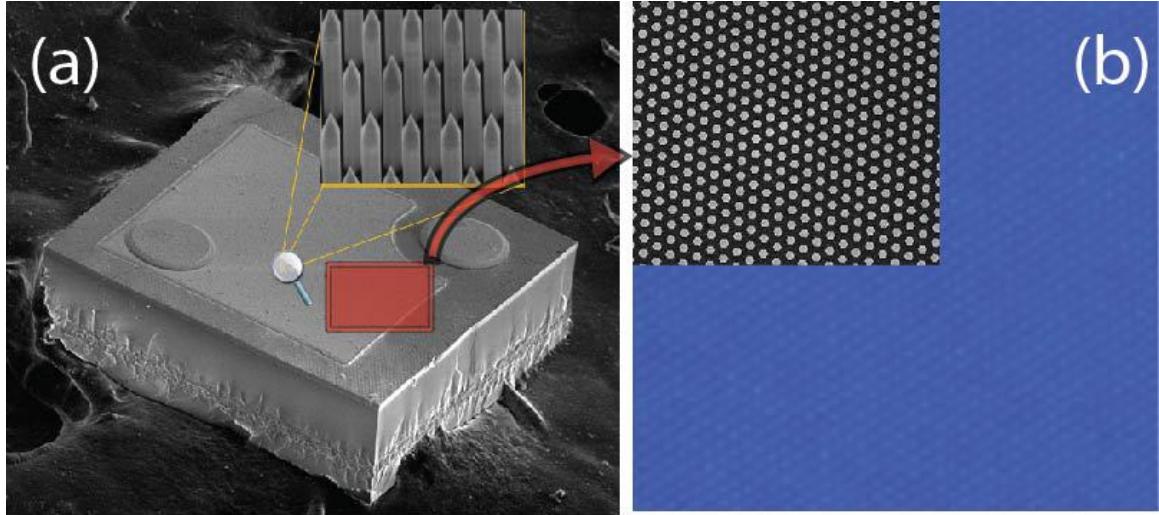


Figure 1.5 (a) SEM of actual glo nanowire chip showing magnified 45 degree view of individual nanowires. (b) The fabricated blue nLED. Each dot represents a nanowire LED. The inset shows top view SEM of nanowire array. Courtesy of glo-USA, Inc.

i.e., Leaky Mode Resonance, Whispering Gallery Modes, Fabry-Perot Resonant Mode and Helical Resonance Modes, Chapter 3 presents our findings for a generalized volumetric modes with light management of sub-wavelength cavities. Chapter 4 presents our methods and findings for calculating band-bending and electronic distribution in both cylindrical and hexagonal core-shell nanowire by solving Poisson-Schrodinger equations self-consistently. In Chapter 5, we apply the inter-band optical transition rates study to understand the extremely enhanced optical properties of hexagonal core-shell nanowires, and rule out three primary factors (overlap integral, oscillator strength and joint optical density of states) which are strong function of dimensionality. The quantum mechanical derivation based on perturbation theory and Fermi's Golden Rule used in this chapter are outlined in more detail in Appendix A. The modeling of lasing threshold based on the optical transition rates in Chapter 6 confirmed that our theoretical explanation, analysis and calculation of optical properties of core-shell nanowire have a very strong dependence on electron confinement. Finally, we present our conclusions in Chapter 7.

Throughout this work we use the term *nanowires* (NWs) to represent a specific quantum confined structure with cross-sections of 2-300 nm and lengths upwards of several micrometers. There are

other research groups using terms such as *nanopillars*, *nanotubes* or *quantum well wires* (QWRs) to discuss the same nanostructures.

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## CHAPTER 2

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### OPTICAL ENHANCEMENT OF CORE-SHELL NANOWIRE

Given that the profound enhancement of optoelectronic properties of nanowires is the major theme of this dissertation, it is dutiful to first summarize the major experimental results, such as fabrication techniques and characteristics of core-shell nanowires (CSNWs).

A CSNW is a quasi-one dimensional structure with a wide band gap materials, such as AlGaAs, wrapping around a low band gap semiconductor, such as GaAs. It is expected that the lower dimensionality of electronic states in CSNW to have a significant influence on both optical and electrical properties of the structure. For instance, electron systems in lower dimensions are adequately treated through perturbation methods, and the correlations among electrons are much more significant due to higher degrees of confinement. The electrons can be moving in the direction of NW growth axis and any small or localized interaction can cause a collective response from the whole system. Importantly, this one-dimensional electron system (1DES) can experimentally be realized in various material systems. These include carbon nanotubes, electrons at the edges of a two-dimensional electron system (2DES), and in NWs.

Electrically it is important account for the electron correlations in order to determine the behavior of the structure. The significant values of exchange and correlation energies in 1DES, makes them an interesting candidate for probing their energy dynamics, and especially the interaction with light. This, however, imposes various experimental challenges and theoretical considerations and will be discussed in the following sections.

## 2.1 Growth of Nanowires

Freestanding quasi-one-dimensional semiconductor NWs based on III-V compound semiconductors, owing to their unique physical properties<sup>107,108</sup>, are considered ideal building blocks for the realization of photonic and electronic nano-scale devices.

Currently, two bottom-up approaches to the fabrication of freestanding nanowires are considered: (i) selective area epitaxy (SAE)<sup>109</sup> and (ii) metal-catalyst assisted growth through the so-called vapor-liquid-solid (VLS) mechanism<sup>110,111</sup>. The latter method relies on the alloying of a metal catalyst (usually Au) nanoparticle with the semiconductor constituent elements, supplied through a vapor phase. The as-formed alloy acts as an initial nucleation site for the material and further guides the nanowire growth, the diameter of the nanowire being controlled by that of the metal nanoparticle<sup>112</sup>.

An advantage of the VLS method over SAE is that it does not require nanolithography processing of the substrate; furthermore, it is compatible with most advanced epitaxial growth techniques for III-V compounds, such as molecular beam epitaxy (MBE)<sup>113,114</sup>, chemical beam epitaxy (CBE)<sup>115</sup>, and metalorganic vapor phase epitaxy (MOVPE)<sup>116,117</sup>. In addition, the growth of epitaxial NWs allows precise control over the material composition and/or intentional doping along the NW length (i.e., growth direction). Most commonly used precursors of group-V elements are arsine ( $AsH_3$ ) and phosphine, however, instead of using the toxic hydrides, the alkyl-substituted arsine and phosphine molecules will be much more safer and improve the materials' electronic properties. The detailed fabrication techniques will be discussed next.

GaAs nanowires were grown by low (50mbar) pressure MOVPE using an Aixtron reactor model AIX200 RD. Trimethylgallium (TMGa) and tertiarybutylarsine (TBAs) were used as gallium and arsenic precursors, respectively. Au nanoparticle deposited on  $(\bar{1}\bar{1}\bar{1})B$  GaAs were used to catalyze the nanowire growth. To this purpose, VGF-grown semi-insulating (undoped) GaAs wafers oriented  $(\bar{1}\bar{1}\bar{1})B$  were used. The substrates were then first degreased in isopropanol vapors, etched in  $4H_2SO_4 : 1H_2O_2 : 2H_2O$  solution for 8 min at around  $40^\circ c$ , rinsed in de-ionized water and finally dried under pure  $N_2$ . Au nanoparticles with  $\sim 60nm$  diameters were prepared by reaction of

$HAuCl_4$  with sodium citrate in aqueous solution and randomly deposited on the as-prepared GaAs surface by dropping a small amount of colloidal solution onto the substrate. The solvent (water) was then evaporated by holding the samples on a hot plate (in air) or a few minutes; Au nanoparticle surface densities thus achieved ranged around  $(1 - 4) \times 10^8 cm^{-2}$ .

After loading the sample into the reactor chamber, its temperature was raised, and sample annealing was then performed for 10 min to absorb GaAs surface oxides and organic residues originating from the Au nanoparticle synthesis. This annealing step would also allow the initial uptake of Ga atoms from the GaAs substrate into the Au nanoparticles. After ramping down the sample temperature to the final growth value, TMGa was admitted to the reactor chamber and the growth was initiated.

## 2.2 Scanning Electron Microscopy Images

The nanowire morphology and dimensions were studied by scanning electron microscopy (SEM) observations using a Dual Beam Scanning Electron/Focused Ion Beam Microscope model FEI Helios; a primary electron beam acceleration voltage of 15 kV and a working distance of 10 mm were employed. Figure 2.1 is top view scanning electron microscopy (SEM) image of nanowires with  $\sim 100nm$  diameter core of GaAs,  $\sim 40nm$  thick of AlGaAs shell, and an additional  $\sim 5nm$  GaAs cap layer. The four figures show the CSNWs array at different magnifications and view angles. These images demonstrate the rather sparse distribution of the wires. In addition, the wires are not fully arrayed with various growth directions and lengths. The most magnified view for the left bottom figure clearly indicate the CSNWs have hexagonal structure and tapering effect along the wire growth direction.

## 2.3 Electrical Characterization of Nanowire

The as-grown CSNWs are used to perform optical characterization measurement. However, in order to measure the CSNWs electrical performance, additional treatments have been taken to make Ohmic contacts between nanowires and transmission lines. Figure 2.2 show the SEM image of one dispersed core-shell nanowire connecting with the transmission line by Focus Ion Beam (FIB) for

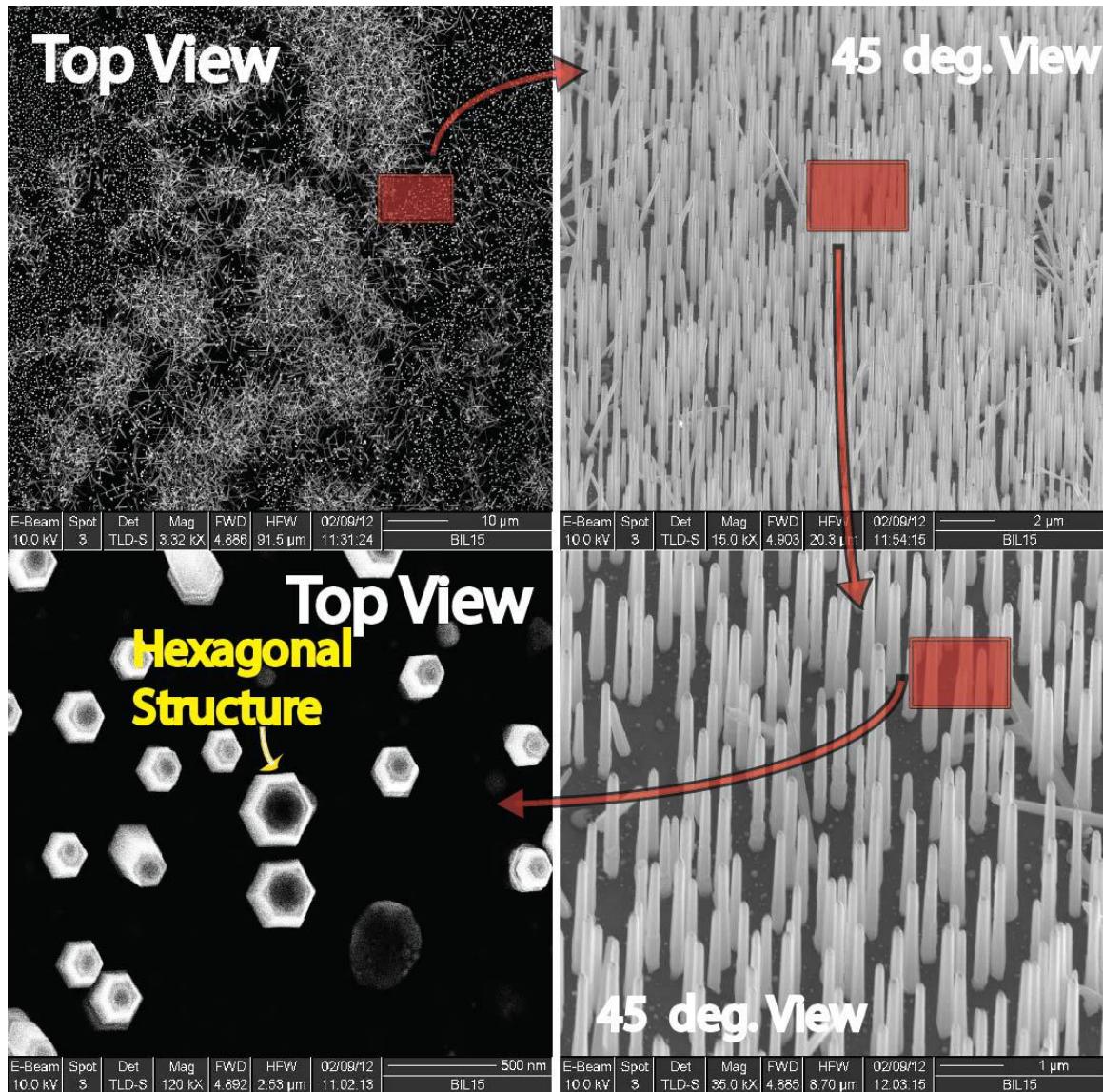


Figure 2.1 Scanning Electron Microscopy image of as-grown GaAs/AlGaAs core-shell nanowires on Si taken at different magnifications and view angles (Image courtesy of Dr.Pouya Dianat)

(left) I-V and (right) C-V measurement. The CSNWs were first detached from the as-grown Si or GaAs substrate by ultrasonication<sup>92,118</sup> in an ethanol bath and dispersed between two transmission lines, then contacted with the transmission lines by FIB using platinum metal.

Characteristic current-voltage (I-V) curves of the nanowire device are given in Fig. 2.3. The experiment is performed with a room-temperature probe station connected with a Keithley 6487 picoammeter voltage source and a network analyzer. The light source is provided by a solar light simulation system with up to  $90\text{ kW/cm}^2$  light intensity. The I-V curve exhibits Ohmic behavior with decreasing of current under higher applied voltage and illumination, confirming that the device is a well-behaved conductor with the electric contact on both sides (Pt) ohmic. The reverse bias dark current of the device is very small,  $\sim 4\text{nA}$  at -10V, and could be further improved by properly passivating the CSNW surface. Upon illumination, the device shows a photo-resistance response due to the excited electron distribution in the CSNW. And this response is magnified with higher bias voltage. Fig. 2.4 shows the capacitance of the device at 1Khz as a function of applied voltage with or without illumination. The metal contact pads of the CSNW device are made large enough to compensate the geometric capacitance as shown in Fig. 2.2(right). The capacitance of this typical device is measured to be  $\sim 20 - 60\text{ pF}$  based on a simple parallel-plate model and thus its cutoff frequency is mainly limited by the transit time of the photo-generated charge carriers in the device, which may in principle reach 100 GHz after certain parameter optimization. With light illumination, the curve fitted capacitance (red line with red dots) increased to 80 pf with a significant transition of capacitance happened at -3.3V. The similar effect also observed in forward bias situation.

## 2.4 Electro-Optically Sampled Time Response

The electro-optic sampling (EOS) set up is shown in Fig 2.5 (a). In essence, the EOS is an ultrafast sampling oscilloscope that uses femtosecond laser pulses to excite optoelectronic transients and then measures the electronic response by probing the refractive index change of an electro-optic crystal placed on top of the device and/or transmission line. In our setup, the laser is split into two paths:

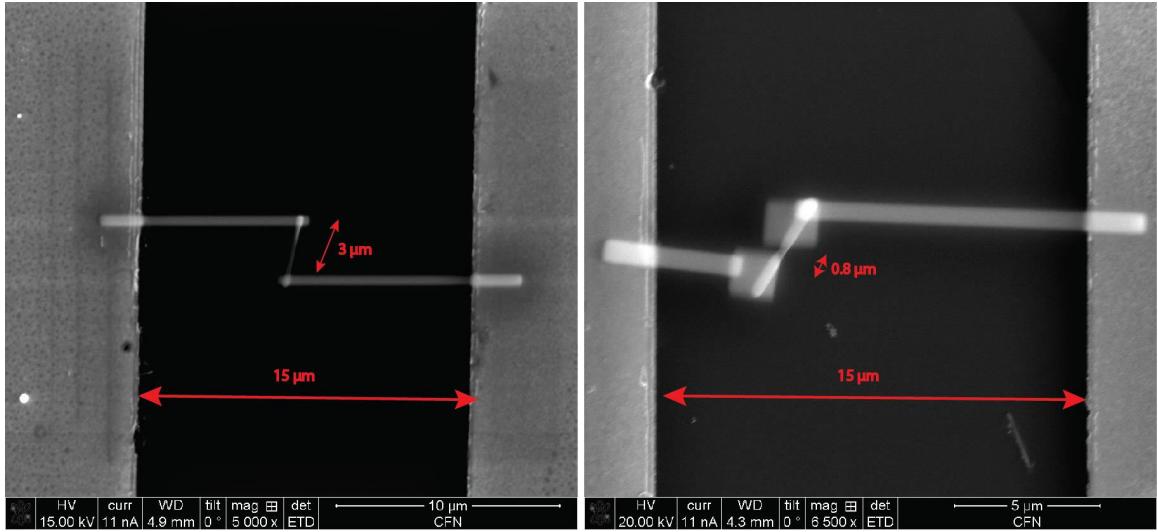


Figure 2.2 Scanning Electron Microscopy (SEM) image of one dispersed core-shell nanowire connecting with the transmission line by Focus Ion Beam (FIB). (left) NW with small contact pad to connect the transmission line for I-V measurement. (right) NW with large contact pad to connect the transmission line for C-V measurement.

one path, the pump beam, is coupled into a fiber to excite the device and the other path, probe beam, passes through a LiTaO<sub>3</sub> crystal to sample the electric field of the propagating response. As shown in Fig. 2.5 (a, b) the CSNW were placed in the middle of a coplanar transmission line (TL), and connected to the TL by Focused Ion Beam (FIB) lithography. The distance between the two FIB contacts is  $\sim 3.5 \mu m$ .

By varying the optical path of the sampling beam, the temporal response of the device is observed with a time resolution limited by the laser pulse width and the response of the electro-optic crystal. The amplitude sensitivity is limited by the noise in our detection system. We modulated the switching beam at 80 kHz and performed phase-sensitive detection with a lock-in amplifier on the light analyzed (with a polarizer and differential detection) from the LiTaO<sub>3</sub> crystal, in order to increase the sensitivity to sub-mV levels. In this experiment,  $\sim 100$  fs pulses from a Ti:sapphire laser with a center wavelength of 830 nm were split into the two paths. The path that is coupled into a fiber to excite the device under test (DUT) is dispersed by the fiber and excites as a 400 fs chirped optical pulse. The second laser path that passes through the LiTaO<sub>3</sub> crystal to sample the propagating

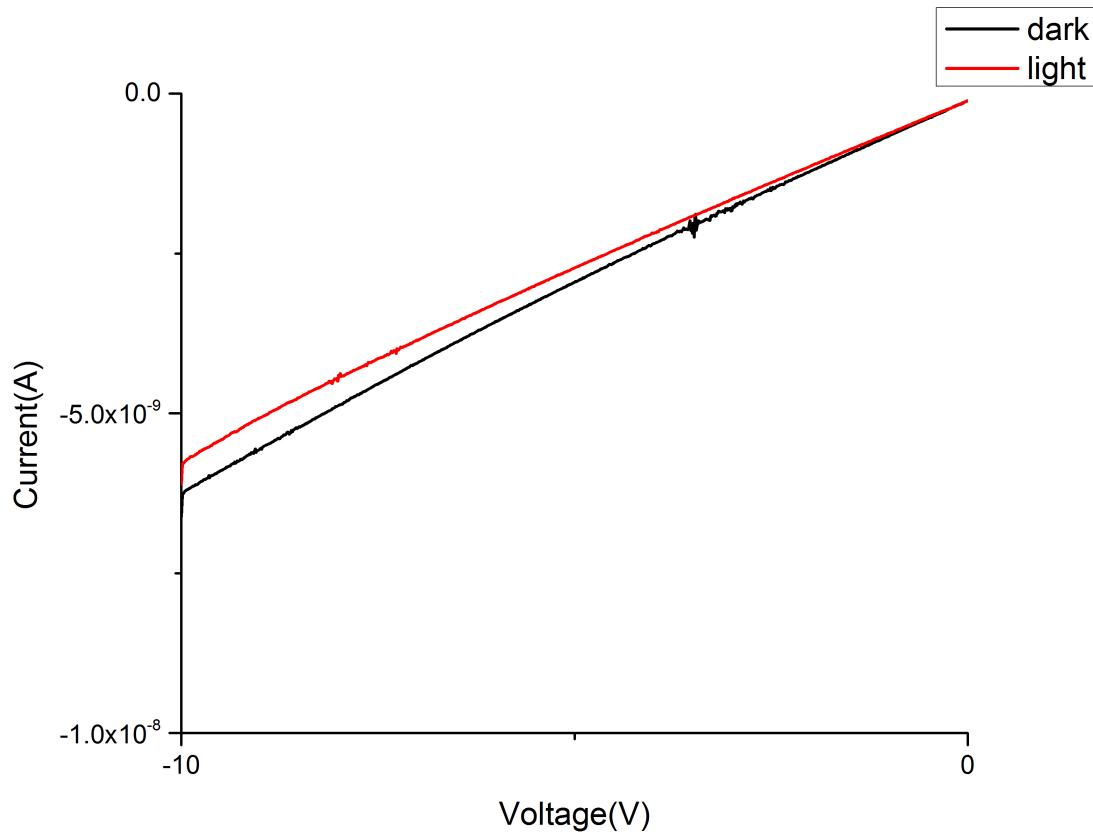


Figure 2.3 Current versus Voltage Measurement under illumination of Single Core-Shell Nanowire.

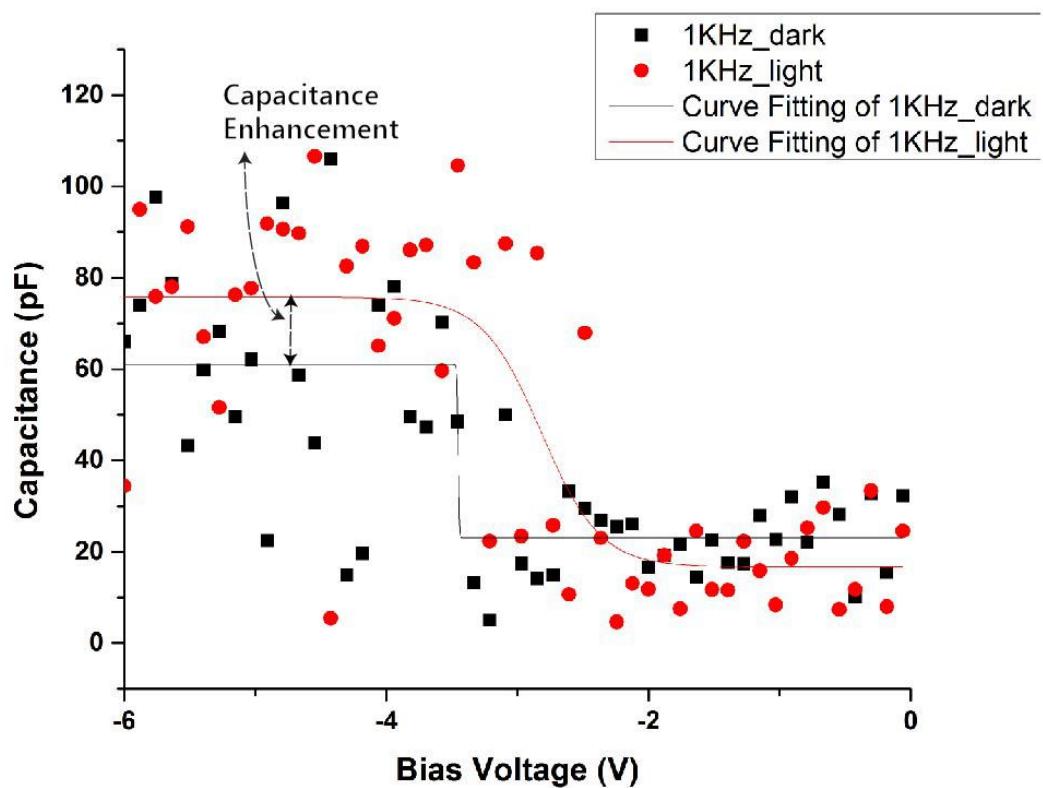


Figure 2.4 Capacitance versus Voltage Measurement under illumination of Single Core-Shell Nanowire.

electric field broadens slightly to a 150 fs optical pulse at the crystal. The photodetectors' electronic response is coupled to a coplanar strip (CPS) transmission line. The separation from the fiber exciting the device to the optical sampling crystal is 250 m. The CPS transmission line is contacted with microwave probes for dc bias and < 50 GHz measurements. Bias values from -10 to +10 V were applied to the CSNW structure with average optical powers ranging from 250 nW to 10 mW. The current – voltage (I-V) measurements in ambient room light (dark) and under continuous wave (CW) illumination by an 830 nm Ti:sapphire laser are performed. The CSNW has very low dark current (<0.1pA) which increases to 170nA average photocurrent with 2.6 mW of optical power; remarkable for a single wire. This corresponds to a responsivity of 0.03 A/W, while the responsivity for the same volume of GaAs in bulk is  $0.02 \times 10^{-3}$  A/W. A three orders of magnitude increase in the responsivity demonstrates that CSNW is not only a good absorber but also converts energy more efficiently compared to their thin film counterparts. This I-V response result shows that the device is an efficient optical detector mostly due to the collection of carriers generated outside of the active region, which are efficiently collected in the low-dimensional electron gas reservoir which will be discussed shortly.

The time response data for the CSNW is shown in Fig. 2.5 (c) under applied bias of 10 V, showing as-measured full-width half-max (FWHM) of ~13 ps. Several factors are involved in the temporal response measured via electro-optic sampling. The overall response comprises three major elements: 1) the device response, 2) the signal propagation, and 3) the electro-optic sampling system measurement. The measurement is a combination of these responses, resulting in a measured signal that is distorted. Thus, the device's intrinsic speed is even faster when the test set up limitations are considered.

Given the length of the wire, this result shows higher speed of both electron and hole transport in the wire. This is due to the electron charge distribution in the core-shell nanowire. Different from the core-only nanowires or bulk semiconductor devices, the CSNWs are able to confine electrons primarily at the hetero-interface of GaAs core and AlGaAs shell, with small amount of electrons

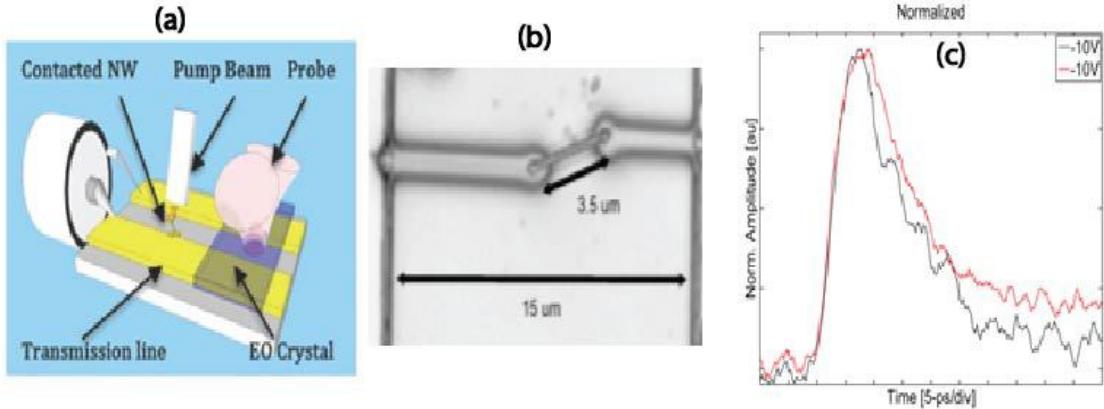


Figure 2.5 (a) Electro-optic sampling (EOS) time response measurement set up: RF probe is at one end of a transmission line in the middle of which the NW is contacted and is excited by 400 fs pulses of light delivered by fiber; probe beam samples the electric field through the electro-optic crystal. (b) Image of the FIB-contacted NWs. (c) Time response data. Image courtesy of Dr. Marc Currie at Naval Research Lab.

in the core. The movement of these charged carriers are confined in two-dimensions, forming a two-dimensional electron gas (2DEG) at the heterojunction. If the CSNW has hexagonal facet more optical excitation produces more electron-hole pairs, and higher order confinement or one-dimensional electron gas (1DEG) will be found as six (6) pillars of charge at the corners of the hexagonal CSNW<sup>119</sup>. In addition to the confined charge carriers' distribution in CSNWs, there is an electric field due to applied bias that moves the optically generated electrons to the 2DEG/1DEG. These optically generated carriers perturb the charge reservoirs, eliciting a collective response that is not limited by the transit of the charges to the contacts. Analogous to a drop exciting a wave in a reservoir that is detected more rapidly than the drop's transport by current flow, charge plasma confined in a semiconductor can transfer energy, hence respond much faster than the electric field-induced carrier drift current.

## 2.5 Optical Characterization of Nanowire

Linear optical spectroscopic techniques, such as absorption, luminescence and modulation spectroscopy, have for a long time been important tools in understanding the basic physics of semi-

conductor devices and materials. Also over the last fifteen years or so, semiconductor optical and optoelectronic properties have become of increasing technological importance in their own right. The ever-growing application of semiconductor diode lasers and related optoelectronic technology in communications and consumer products has helped to give yet further impetus to research on semiconductor optical properties.

### 2.5.1 Absorption Enhancement

Figure 2.6 shows the reflectivity of a GaAs wafer on which 50 nm thin film of AlGaAs is grown, and compared this to the reflectivity spectrum of a Si substrate. As expected, about 30% to 55% of a normally incident light is reflected in bulk Si and GaAs, with a sharp change for wavelengths near their respective band gaps. All the data are normalized to the reflectivity of gold (Au).

Figure 2.7 contrasts this with the measured absorption spectrum of two types of GaAs core, AlGaAs shell nanowires (CSNWs): those grown on a GaAs substrate (black), and the others heteroepitaxially grown on a Si substrate (red). The spectra show that both cases have the signature change of reflectivity at badgap of GaAs, i.e., these are due to the GaAs/AlGaAs CSNWs, not the substrate. Importantly, for the wavelength range of 700-1200nm these core-shells which only occupy 15% of the volume compared to thin films of the same height, reflect 2-4% of light for the CSNWs grown on Si, and 3-7% of light for those grown on GaAs substrate. The beam-width of the incident light being  $\sim 1\mu m$ , this shows that only a few NWs are interrogated by light and, normalized to volume, these wires absorb more than two orders of magnitude more light than their thin-film counterparts.

### 2.5.2 Emission Enhancement

Figure 2.8 compares room temperature micro photoluminescence (PL) spectrum of bulk GaAs to CSNWs grown on GaAs, and two cuts of Si. The ratio of peak luminescence of a) CSNWs on GaAs, B) CSNWs on Si[111] and c) Si(miscut) substrates to bulk GaAs are, respectively, 923, 311 and 10. Considering the beam width of  $\sim 1\mu m$ , 5-10 NW were excited, yet emitted over three order of magnitude more light compared to bulk.

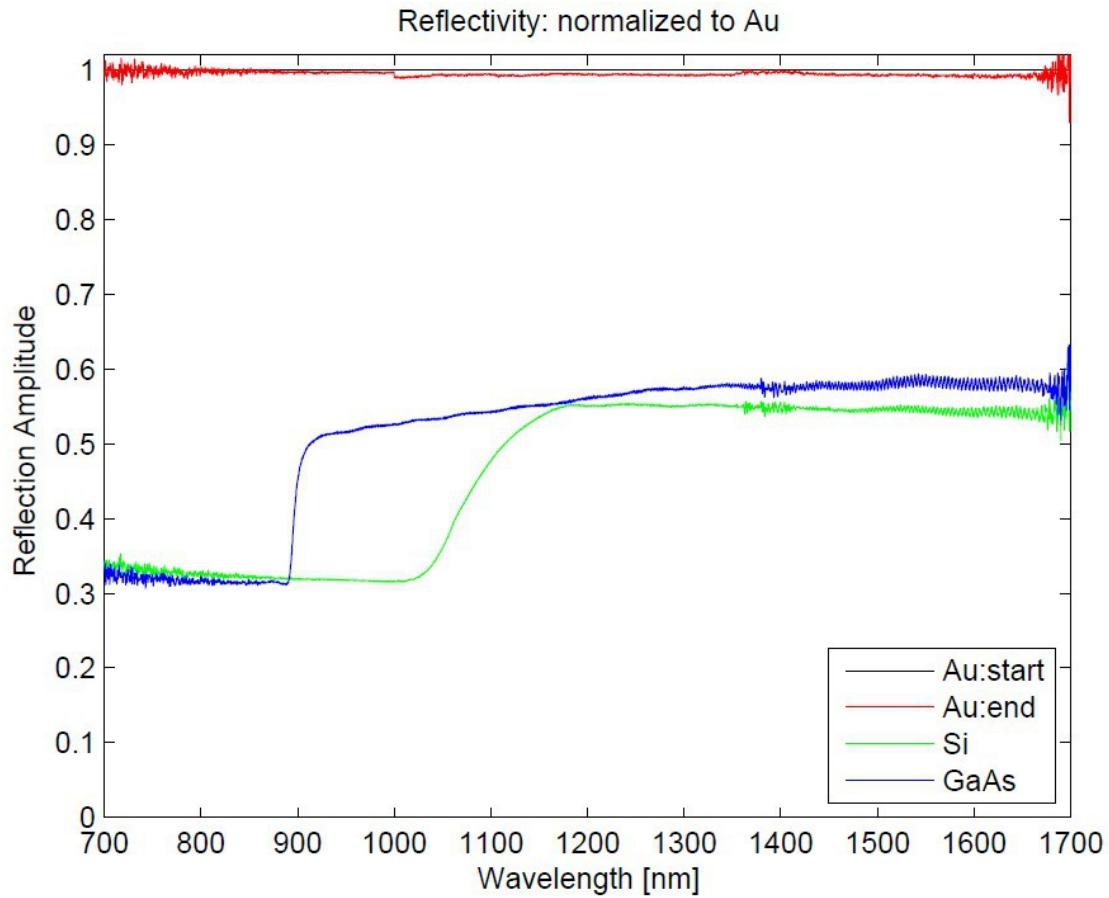
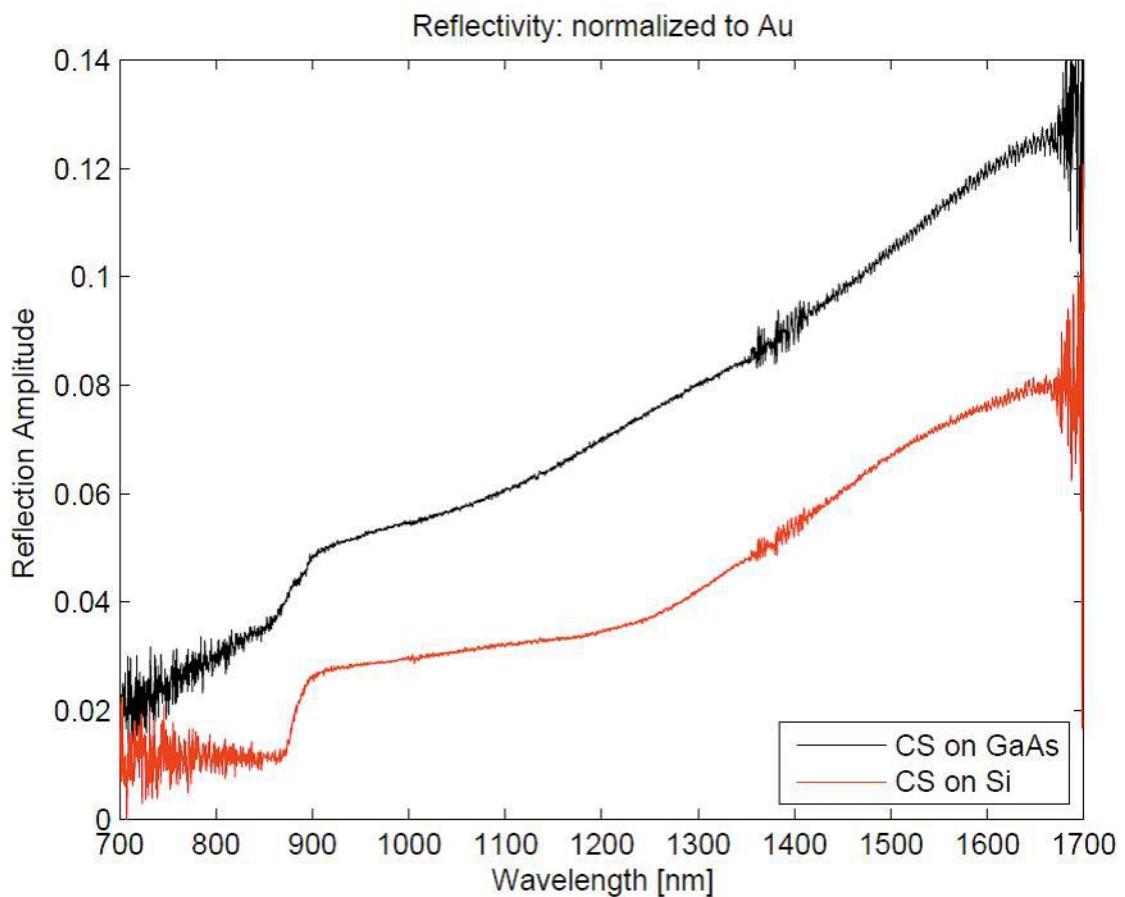


Figure 2.6 Reflectivity of GaAs (blue) and Si (green) substrates measured with  $\sim \mu\text{m}$  normally incident beam.



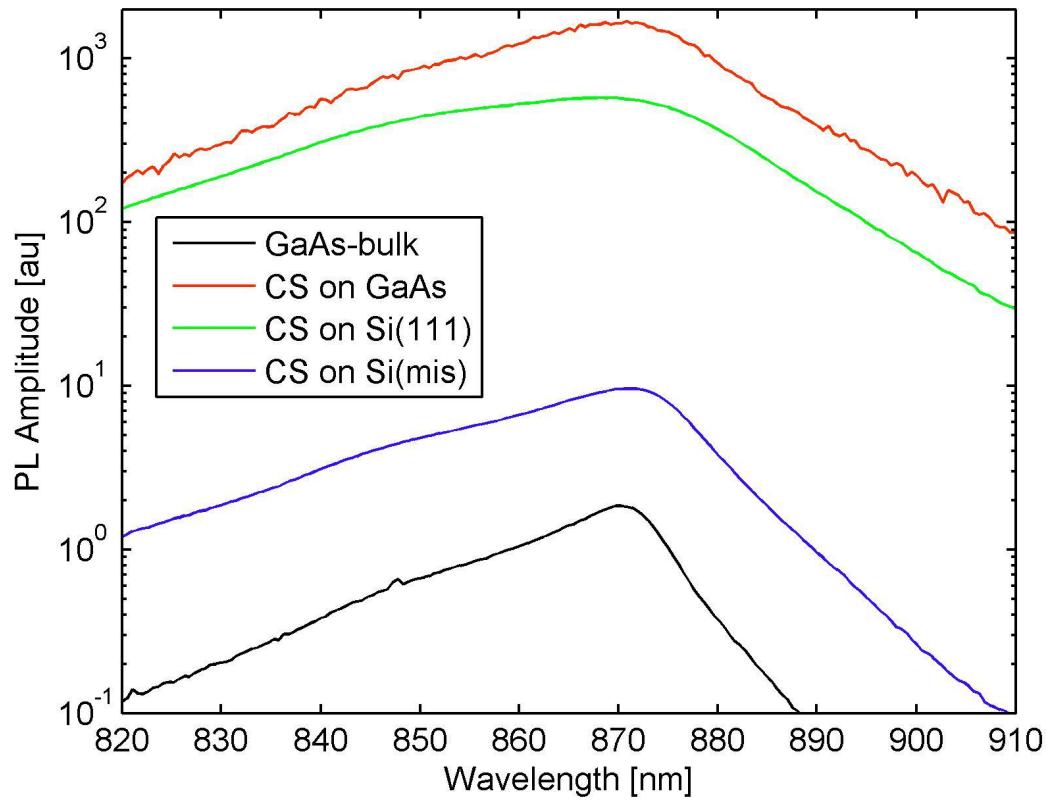


Figure 2.8 Photoluminescence of bulk GaAs, Core-Shell Nanowires grown on GaAs and Si.

### 2.5.3 Lasing

Photoluminescence (PL) of bulk GaAs to CSNWs grown on GaAs, and on two directions of Si showed that normalized to the fraction of the volume that these wires occupy, nearly 10,000 times more brightness is observed in these wires compared to thin-film as in Fig. 2.8. In the case of stimulated emission of light, the photon mode density ( $1 + u_\varepsilon$ ) plays a crucial role. Figure 2.9 is the photoluminescence (PL) spectrum at various optical pump intensities. As the excitation laser power increase beyond  $5\mu W$  a sudden and highly nonlinear increase in the emission intensity is observed, with pronounced peaks emerging from 800nm to 850nm that rapidly grows to become several orders of magnitude stronger than the background emission. The lasing amplitude versus excitation power demonstrates a threshold of around  $5\mu W$ , followed by saturation near  $12\mu W$ . This nonlinear threshold behavior shows in detail in the L-L plot, (i.e., The pumping power intensity ( $L$ ) versus output light power intensity ( $L$ )) as in Fig. 2.10. The sharp peak has a full width half maximum (FWHM) that varies from 1.5 to 3.5 nm. This remarkable behavior is achieved in the as-grown wires with no vertical structure.

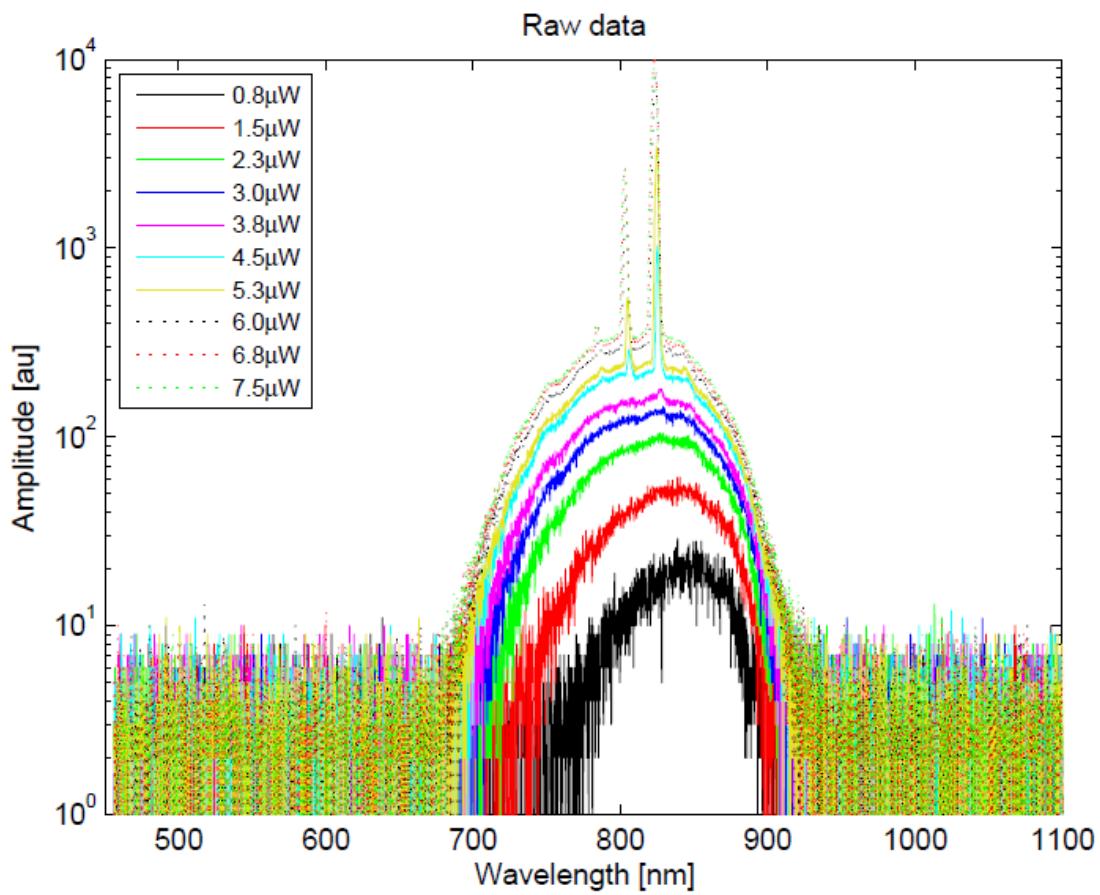


Figure 2.9 Micro-Photoluminescence measurements with fs-pulsed, 532-nm laser excitation at 250kHz repetition rate shows lasing of the as-grown wires.

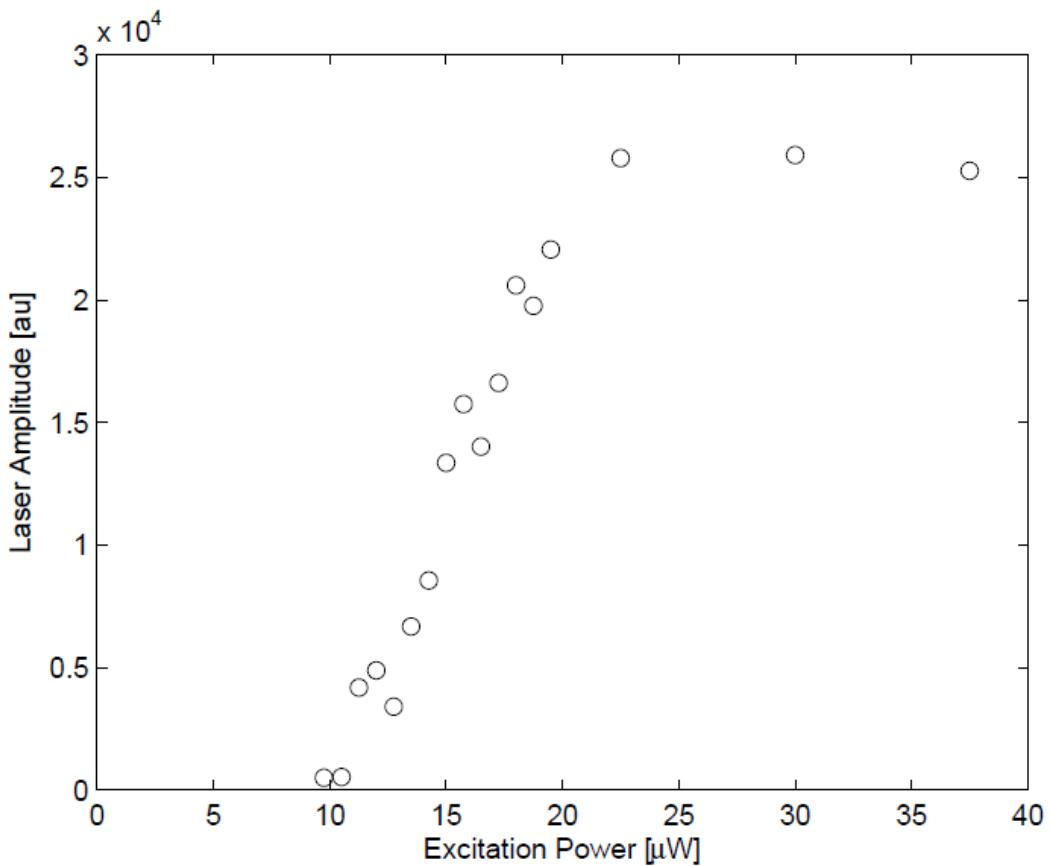


Figure 2.10 *L-L* curve of as-grown core-shell nanowire. The pumping power intensity (*L*) versus output light power intensity (*L*) of as-grown core-shell nanowire operating at room temperature with a low threshold of  $\sim 10\mu W$  and followed by saturation near  $22\mu W$ .

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## CHAPTER 3

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### LIGHT CONFINEMENT IN SUB-WAVELENGTH NANO-STRUCTURE

#### 3.1 Light and Nanowire

##### 3.1.1 Leaky Mode Resonance

Interaction of light with a dielectric or metallic cylindrical medium is analyzed by solving Maxwell's equations with the appropriate boundary conditions in the classical waveguide theory<sup>120</sup>, which leads to highly confined modes in optical fibers and microscale dielectric resonators. In an infinitely long cylinder, even at deep sub-wavelength diameters this results in a characteristic equation, the solution to which are the transverse magnetic (TM) and transverse electric (TE) resonant modes. We can define the electromagnetic modes of localized resonators as time-harmonic solutions of the form  $\mathbf{E}(\mathbf{r}, t) = \mathbf{E}(\mathbf{r}, \omega)e^{-i\omega t}$  to the source-free Maxwell equations. This solution shows that the longitudinal field component distributes outside the NW and is in resonance with the natural modes, such as  $TE_{11}$ ,  $TM_{02}$ , etc., supported by the NW. These modes have been termed leaky-mode resonances (LMR)<sup>29,121</sup>, and provide an intuitive tool to facilitate the understanding and optimization of the resonance effect in such nano-structures.

We replicate these results using MEEP, a widely used open-source finite-difference time-domain (FDTD) simulation package<sup>122</sup>, to identify how light is confined in an infinitely long GaAs nanowire. The top row of Fig. 3.1 shows several configurations of TM LMR modes for a NW with diameter of 220 nm, with excitation single wavelength light being incident parallel to the NW axis. The blue and red color codes represent the polarization of the electric fields. The TE modes are primarily

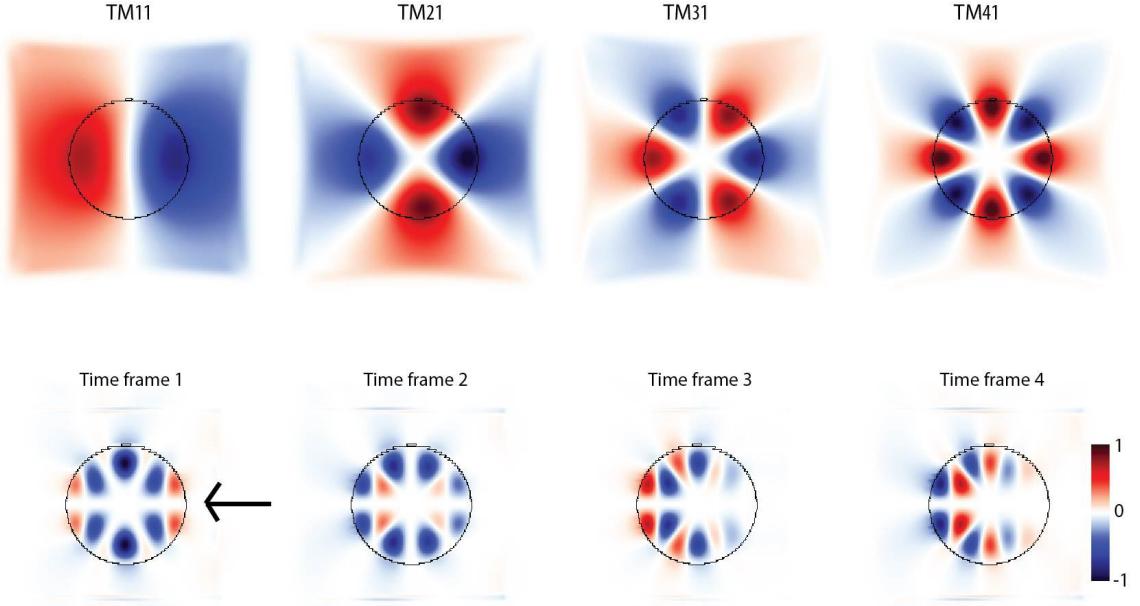


Figure 3.1 (Top) Resonant modes in an infinitely long cylinder of GaAs with diameter of 220 nm with light incident parallel to NW axis. (Bottom) The Poynting vector at different time frames with light incident perpendicular to the NW axis from the right.

identical to the TM modes shown here with the electric and magnetic fields exchanged. If the light is incident with an arbitrary angle, then so-called hybrid HE and EH leaky modes will be excited instead of the pure TE or TM mode. The bottom row of Fig. 3.1 shows the directional energy flux density of the electromagnetic field, the Poynting vector, at different time frames with light being incident perpendicular to the NW axis from the right side. The light is seen to propagate from the right and then mostly remain confined at the left part of the cylinder. It is notable that in either case the light energy is spatially distributed along the cross section of the wire but, as expected from a 2D treatment does not vary axially. Figure 3.1 demonstrates that the LMR can gently confine light within subwavelength semiconductor nano-structures, similar to the intuitive ray-optics picture of multiple total internal reflections from the periphery of the cylinder. As shown by in Ref. <sup>29</sup>, these LMRs depend on the radius and the height of the dielectric, which allows light engineering of the nanowires so as to increase its absorption efficiency at pre-determined wavelength, e.g., to maximize absorption of sunlight spectrum for higher efficiency solar cells, or to radiate as optical antennas.

### 3.1.2 Whispering Gallery Modes

Infinitely long cylindrical or hexagonal NW structures can also support Whispering Gallery (WG) modes<sup>1,98,123–129</sup>. To calculate the resonant WGMs, Maxwell's equations have to be solved numerically<sup>130</sup> taking into consideration the spectral dependence of the material of interest's index of refraction. However, we can deduce a simple plane-wave model from theoretical derivations, and the relationship between resonance wavelength  $\lambda$  and the corresponding mode serial number  $N$  can be obtained<sup>129</sup>. The WG modes can also reflect and confine light in the (subwavelength) nanostructure by total internal reflection from the curvature of the structure boundaries. However, a light wave can interfere with itself only when having completed one full circulation within the resonator, which means only the light with one or multiple wavelengths are allowed to perform multiple circulations generating a standing wave. Figure 3.2 from reference<sup>1</sup> shows near-field intensity patterns of low-order TM polarized hexagonal WGMs for  $n = 1$  and refractive index  $n_r = 2.1$ . Each mode pattern is labeled by its respective mode number  $m$  (lower right number) and its symmetry class (upper right symbol).

For comparison, four mode patterns of the circular cavity are given in the upper left and lower right together with their angular mode number. We again observe the radial spatial dependence of light intensity. Furthermore, the low order WG modes of hexagonal NWs are essentially similar to the cylindrical ones, but for higher order modes additional features will arise on the facets of the hexagonal NWs<sup>1</sup>. Simulation results also show little difference between WG mode and Leaky modes in lower order modes for both hexagonal and cylindrical structures. As with the LMR, the resonant WG modes have been used as the basis for a precise theoretical explanation of the enhanced optical behavior of hexagonal NWs, such as enhanced light absorption<sup>29,62,131–133</sup> and emission<sup>31,123,134,135</sup>. Furthermore, these numerical solutions have led to reproduction of experimental resonance spectra, e.g., polarization-resolved micro-photoluminescence (-PL) and cathodeluminescence (CL) spectroscopy.

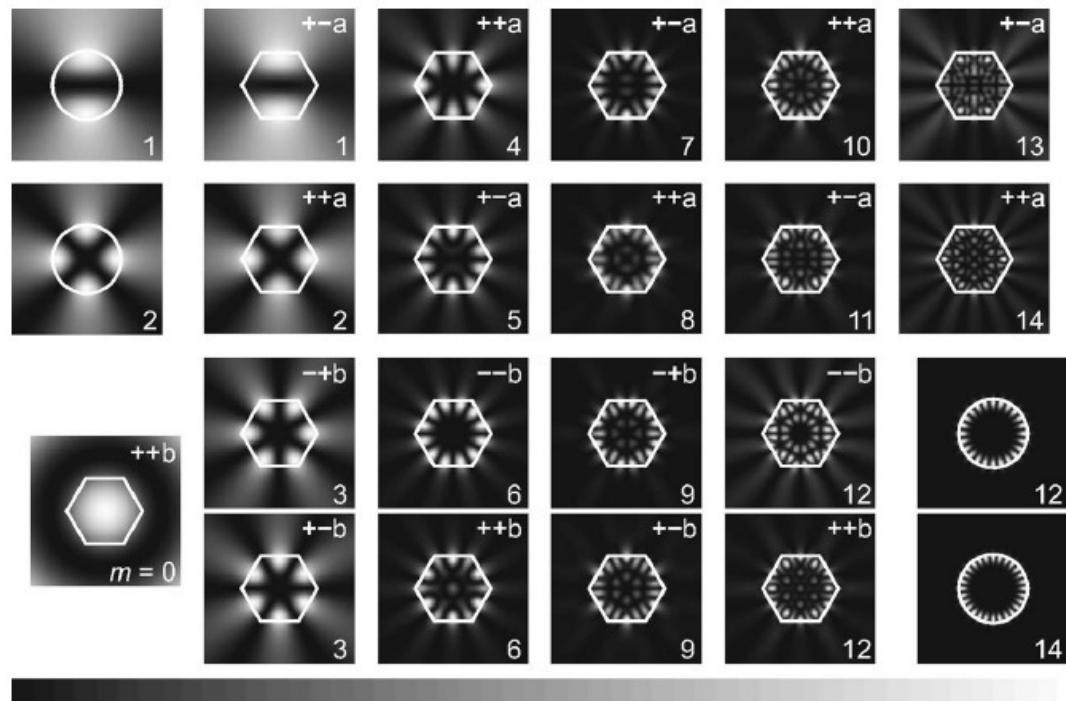


Figure 3.2 Several configurations of Whispering Gallery resonance modes in infinite long cylindrical and hexagonal nanowire. For comparison, four mode patterns of the circular cavity are given in the upper and lower right together with their angular mode number. (Reprinted with permission from<sup>1</sup>, ©2005 by the American Physical Society.)

### 3.1.3 Fabry-Pérot Resonant Mode

The above analysis and results apply to long structures, hence, provide two-dimensional radial modes, independent of the NW axis. However, light confinement has strong axial dependence, necessitating three-dimensional analysis of the cavity modes. FDTD simulation in 3D are used to identify the axial dependence of resonant modes in these nano-structures, revealing modes which are volumetric in nature.

Fabry-Pérot (FP) modes have been analyzed for sub-microcavity, or nano-cavity, NWs with cylindrical or hexagonal structures, specifically in order to determine the axial dependence of the resonance modes <sup>136</sup>. At least two mirrors are needed to construct the reflection structure inside the cavity, whether they are the top and bottom ends, i.e., the air and substrate interfaces with the nanowire, or any of the two opposite facets along the nanowire axis. For subwavelength structures, the longitudinal WG modes have high scattering losses due to diffraction, and axial FP waveguide modes will dominate<sup>128</sup>. However, due to small difference of the refractive index between the substrate and the nanowire dielectric, the existence of the FP mode will only be valid if the nanowire has relatively large radii, e.g., larger than 200 nm<sup>137</sup>. Under these conditions, besides the top and bottom ends, the lateral facets of nanowire can also be treated as two parallel slabs, and with the dielectric in between, it can support the FP mode with mode spacing inversely related to the nanowire length. An application of this analysis is in the design of NW lasers, since the optical cavity modes are observed at threshold for lasing, and have been investigated for both optical and electrical pumped cases <sup>34,138</sup>. As a results the FP resonance mode based nanoscale lasers are not only capable of covering a wide spectral regions, but can also can be integrated as single or multi-color laser source arrays in silicon based photonic integrated circuit or microelectronic devices <sup>34,138</sup>. However, the FP modes supported by the nano-cavity structure have relatively small quality factor due to the small difference of the refractive indices of the substrate and the NWs. In order to address this issue, Bragg gratings can be produced at the NW ends, alternatively, NWs can be placed on metal substrates in order to increase the FP resonance peak intensity by more than one order of magnitude

compared to those on Si substrates<sup>139</sup>.

### 3.1.4 Helical Resonance Modes

Nanoneedles of III-V material grown on heterogeneous substrates are optoelectronic devices which have shown interesting optical behavior, including lasing, at room temperature<sup>2</sup>. Figure 3.3 (a) shows SEM image of a nano-laser grown on silicon substrate that has subwavelength dimensions on all sides. Analysis of light propagation introduced by shows that unlike the traditional WG mode that lack vertical structure, there is net propagation in axial direction in these structures which leads to volumetric resonant modes which are termed helical mode resonances<sup>2</sup>. The schematic Fig. 3.3(b) suggests a helical ray path with nearly total internal reflection at the nanopillar-silicon interface due to the glancing angle of incidence from the hexagonal facets of the nano-laser shown in Fig. 3.3(a). As such, the faceted shape of the structure affects the optical cavity properties. FDTD-simulated field profile shows a hexagonal WG-like mode pattern in the transverse plane as in Fig. 3.3 (c), which arises from strong azimuthal components of helical modes. Figure 3.3 (d) shows first-order and higher-order standing waves axial variation. The radial mode number (first number, m) describes the transverse field pattern for WG modes, and the axial mode number (second number, n) describes the axial standing wave as is the case for Fabry-Perot resonances. It is seen that light or optical field can be well confined in the nanostructure even with low index contrast at the dielectric interface thus producing the nano-resonators needed for lasing. Although the quality (Q) factors of such nanostructure are usually not large, these helically propagating cavity modes, provide an optical feedback mechanism without the sophisticated mirror structures of the vertical cavity surface emitting lasers (VCSELs). Additionally, since the nanowires are heteroepitaxially grown on different substrates, they enable heterogeneous integration of photonic emitters and silicon based computational circuitry. Whereas traditional FP modes are inhibited by the interface between semiconductor nanostructure and the silicon substrate, such unique optical structures have been proposed as an avenue for engineering and integrating on-chip nanophotonic devices.

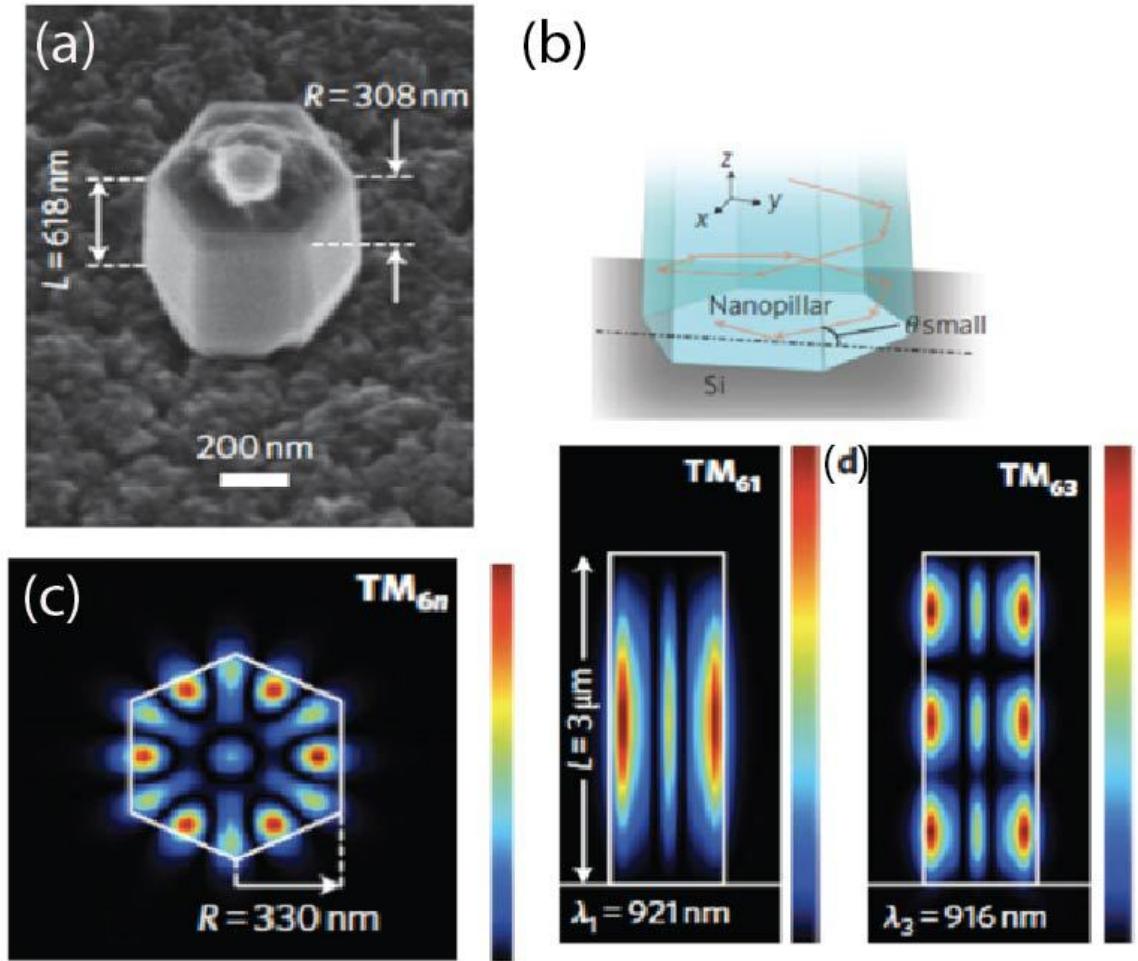


Figure 3.3 Helically propagating modes for optical feedback. (a) SEM image of the nanolaser grown on silicon substrate. (b) Schematic depicting a helical ray path because of glancing angle of incidence from the hexagonal facets of the nanolaser shown in (a). (c) FDTD-simulated field profile shows a hexagonal WG-like mode pattern in the transverse plane, which arises from strong azimuthal components of helical resonance modes. (d) First-order and higher-order standing waves' axial variation. (Reprinted with permission from Macmillan Publishers Ltd: Nature Photonics<sup>2</sup>, ©2011)

## 3.2 Volumetric Modes

### 3.2.1 FDTD Simulation

The finite-difference time-domain (FDTD) algorithm is one of the most common computational tools in classical electromagnetism, which divides space and time into a regular grid and simulates the time evolution of Maxwell's equations<sup>140,141</sup>. The starting point for any FDTD solver is the time-derivative parts of Maxwell's equations, which in their simplest form can be written:

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} - \mathbf{J}_B \quad (3.1)$$

$$\frac{\partial \mathbf{D}}{\partial t} = +\nabla \times \mathbf{H} - \mathbf{J} \quad (3.2)$$

where  $\mathbf{E}$  and  $\mathbf{H}$  are the macroscopic electric and magnetic fields, respectively.  $\mathbf{D}$  and  $\mathbf{B}$  are the electric displacement and magnetic induction fields<sup>142</sup>, respectively.  $\mathbf{J}$  is the electric-charge current density, and  $\mathbf{J}_b$  is a fictitious magnetic-charge current density which used for the calculation convenience of magnetic-dipole sources. In time-domain calculations, one typically solves the initial-value problem where the fields and currents are zero for  $t < 0$ , and then nonzero values evolve in response to some currents  $\mathbf{J}(\mathbf{x}, t)$  and/or  $\mathbf{J}_b(\mathbf{x}, t)$ . However, the frequency-domain solver assumes a time dependence of  $e^{-i\omega t}$  for all currents and fields, and solves the resulting linear equations for the steady-state response or eigen-modes<sup>143</sup>.

In this chapter, all the simulation work were carried out by an open-source simulation package MEEP (an acronym for MIT Electromagnetic Equation Propagation)<sup>122</sup>, which implemented the FDTD algorithm. The advantages of MEEP compared to other commercially available FDTD software packages are: free and open-source which extends the flexibility provided by access to the source code. In addition, MEEP is full-featured, including: arbitrary anisotropic, nonlinear, and dispersive electric and magnetic media; a variety of boundary conditions including symmetries and perfectly matched layers (PML); distributed-memory parallelism; Cartesian (1d/2d/3d) and

cylindrical coordinates; and flexible output and field computations.

In order to perform the simulation in 2D by MEEP, a core-shell hexagonal structure has to be constructed using cylindrical coordinates as in Fig. 3.4, which takes the advantages of geometric symmetries to reduce the computation time. The radius of AlGaAs shell is 185 nm, and the radius of GaAs core is 40% of the shell, i.e., 74 nm. The dielectric constant for GaAs and AlGaAs sets to be 3.4 and 3.3, respectively. Air with unit dielectric constant fills between this hexagonal structure and the perfectly matched layer (PML). The PML is an artificial absorbing layer used to truncate computational regions with open boundaries for solving electromagnetic wave equations numerically. The primary difference between PML and an ordinary absorbing materials is that the waves incident upon the PML from a non-PML medium do not reflect at the interface, thus, allow the PML to completely absorb outgoing waves from the interior of a computational region without reflecting them back into the inner region. Finally, a Gaussian pulse source at the right corner of the hexagon with certain center frequency and bandwidth is used to excite the structure. The simulation stops until the sources are finished, and then to run for some additional period of time. In that additional period, the electromagnetic field is processed at a specific point to identify the frequencies and decay rates of the modes excited.

3D simulation can be easily performed by adding one additional degree of freedom which is the nanowire length. The simulated cylindrical and hexagonal structures with cylindrical coordinates sketch at the bottom of Fig. 3.5 (a). The top row of Fig. 3.5 (a) shows the transverse plane mode for cylindrical (left) and hexagonal (right) core-only NW which is a cross-section cut at the center of the wire. The middle row depicts the longitudinal plane mode for cylindrical and hexagonal structures. These results are transverse magnetic (TM) resonance modes adapted from a single time frame of the electromagnetic evolving in the NW structure with respect to time. Figure 3.5 (b) shows the 3D view of electromagnetic field distribution at the middle of a hexagonal NW. The electrical field is tightly confined at the corners and facets of the structure with a little light at the core.

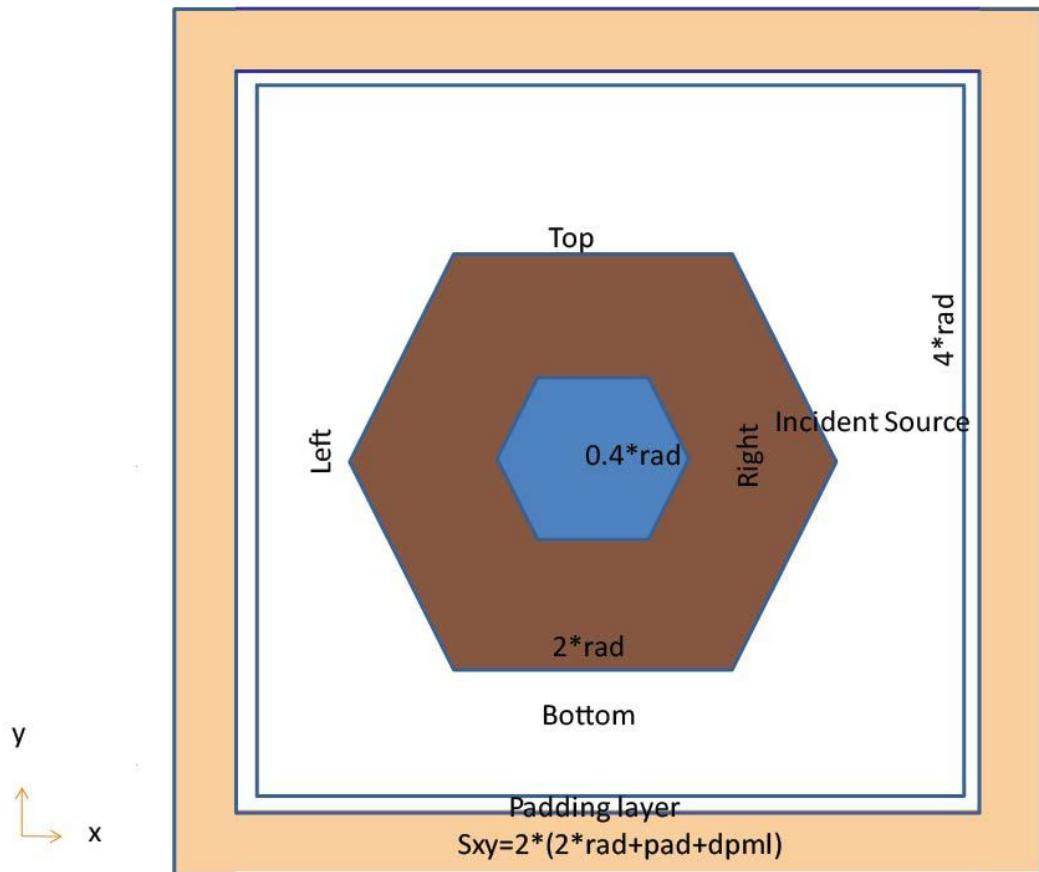


Figure 3.4 A schematic illustration of Finite-Difference-Time-Domain (FDTD) Simulation Set Up.

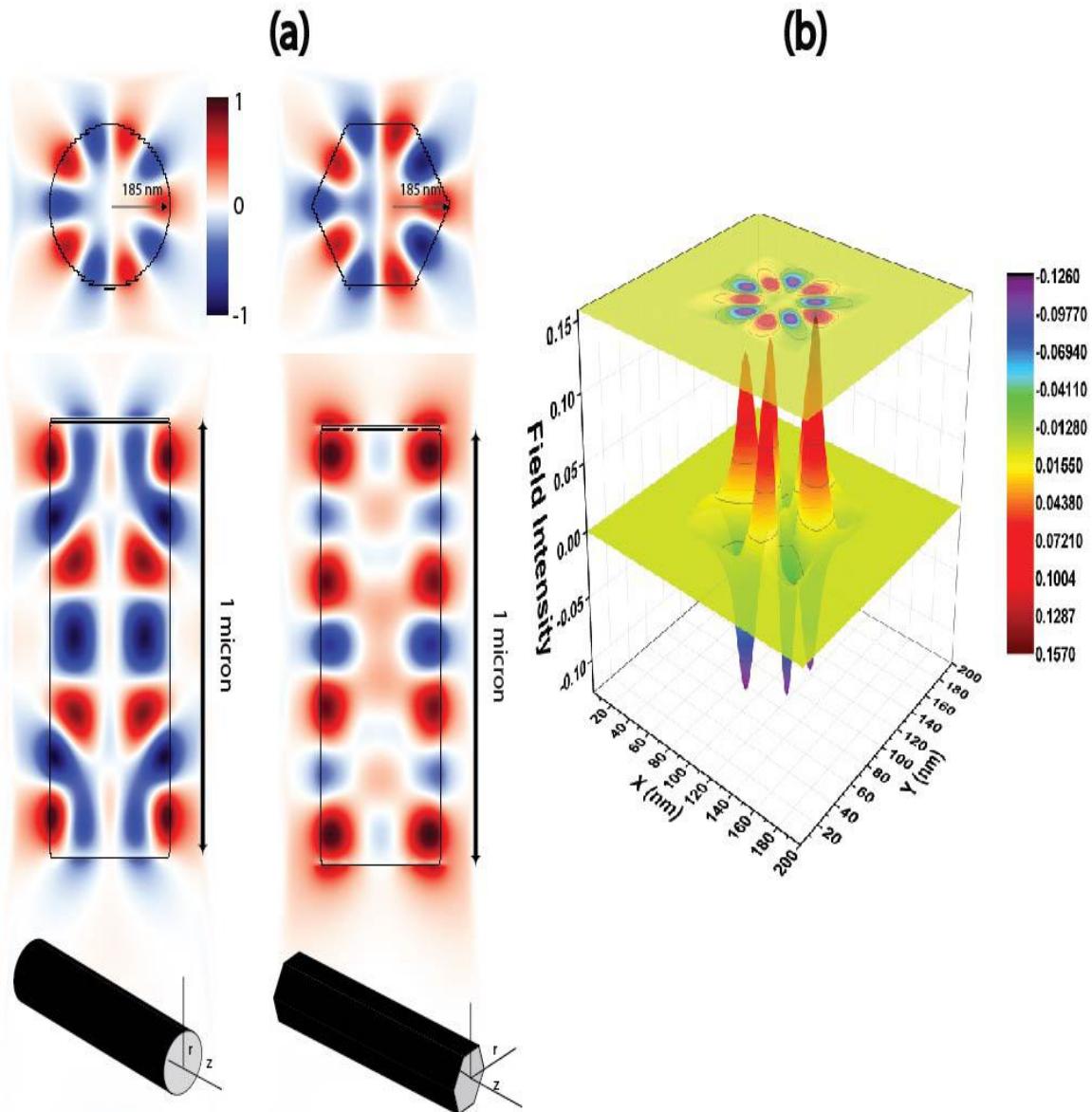


Figure 3.5 (a) (top) Transverse plane mode for cylindrical and hexagonal core-only nanowire. (middle) The corresponding longitudinal plane mode. (bottom) Three dimensional simulation schematic for cylindrical and hexagonal nanowires. (b) 3D view of electromagnetic field distribution at the middle of a hexagonal NW.

### 3.2.2 Generalized Volumetric Modes

The diameter of the nanostructures which can support the helical resonance modes is near the Rayleigh limit, around the boundary of the validity of ray-optics. FDTD analysis can be applied to deeper subwavelength structure in order to identify the cavity modes which are by nature volumetric, i.e., axially dependent. Figure 3.6 shows simulation results for various diameters of hexagonal structure of 1  $\mu\text{m}$  length. Incident radiation with 532 nm wavelength is nearly parallel to the wire axis and different modes are displayed for different radii. Top row shows radial spatial dependence at the middle of the wire axis, and the bottom row shows the axial dependence. Top row results are similar to Figures 3.1 and 3.2, and the bottom row shows that the light can be confined in volumetric resonance mode in both transverse plane and longitudinal plane even with sub-wavelength diameter of these hexagonal NWs. Unlike helical modes, the explanation of resonance need not rely on an intuitive ray-optics description based on the grazing angle of incident light, but shows similar results in how the deep subwavelength structures can confine the light and produce a resonant cavity without having sophisticated mirrors at the end facets. In this respect nano-cavities of as-grown nanowires outperform microcavities of VCSELs.

The same results that are obtained from hexagonal NWs apply to cylindrical ones as shown in Figure 3.10, which compares the simulation results for cylindrical and hexagonal core-only and core-shell NWs with cylindrical coordinates  $\mathbf{r}$ ,  $\mathbf{z}$ . Since these nano-cavities resonances have net propagation in the axial direction, two distinct mode numbers  $m$  and  $n$ , such as in  $\text{TM}_{m,n}$ , are used to describe the azimuthal mode and axial mode, respectively. The transverse magnetic resonant mode  $\text{TM}_{5,7}$  with electric field perpendicular to the nanowire axis is shown for circular (Fig. 3.10 (a), (b)) and hexagonal (Fig. 3.10 (c), (d)) cross-sections. Top row of Fig. 3.10 are the radial standing wave patterns taken at the middle of the NW, and bottom parts are the axial variation which together demonstrate standing wave patterns in the nano-cavity. The hexagonal and cylindrical NWs present nearly identical optical behavior if the nanowires have the same cross-sectional area, consistent with previous findings<sup>144</sup>. These simulations produce the same results as the two-dimensional analysis

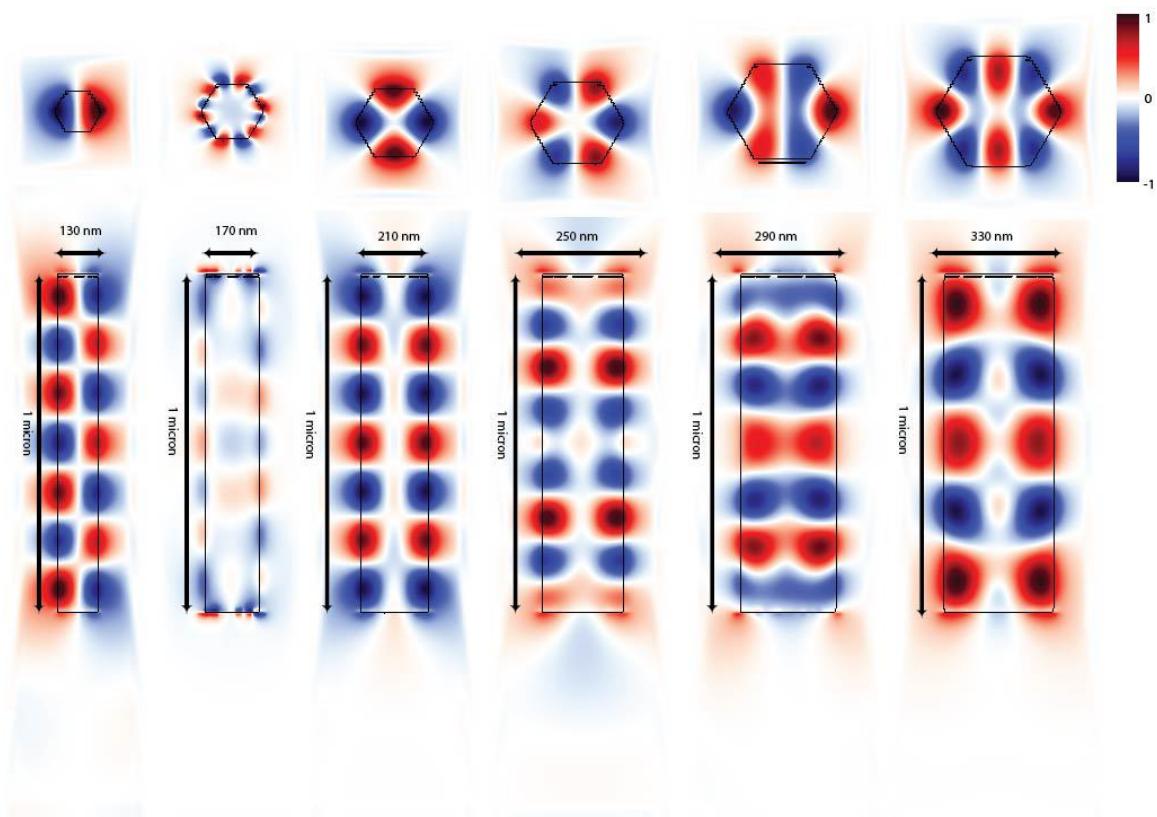


Figure 3.6 Volumetric cavity modes' dependence on nanowire diameter. Top row is a radial cut at the middle of the wire, bottom row is the corresponding axial spatial variation.

of Leaky Modes and Whispering Gallery, as well as the volumetric analysis presented in terms of Fabry-Perot and Helical resonance modes. The results indicate, however, that there is no need for light to reflect from the parallel facets of the wire as in the last two descriptions, rather, the curved surfaces in the sub-wavelength structure can confine the light equally well.

### 3.2.3 Geometry Dependence

Both the materials and the geometric parameters of the core-shell nanowires can be easily controlled by the chemical compositions and/or the temperature/reaction rates during the growth process. Figure 3.7 and 3.8 show the FDTD simulation results for both transverse plane and longitudinal plane modes for cylindrical and hexagonal CSNWs at same wavelength (532 nm) of incident light, respectively. The left part of Fig. 3.7 and 3.8 is air-core/AlGaAs-shell, while the right part is GaAs-core/AlGaAs-shell. And they vary with different core/shell radius ratios, i.e., (top)  $r_{core} = 40\% r_{shell}$  (middle)  $r_{core} = 60\% r_{shell}$  and (bottom)  $r_{core} = 80\% r_{shell}$ . As expected, a core with unit dielectric constant will confine the light more into the shell. The reduction of the shell thickness will further move the light into the shell with a little light in the core. However, in the right part of Fig. 3.7 and 3.8, the results clearly indicated that the increasing of the core-shell radius ratio does not modify the electromagnetic field distribution inside of the CSNWs. The transverse plane modes keep the same mode number, as  $TM_{5n}$ , for different ratios. In addition, the materials variation does not alter the mechanisms of confinement of light in the CSNWs, but only a shift of the resonance frequency corresponding to the dielectric constant and the bandgap of the materials.

In Fig. 3.9, the diameters and the length dependence of the CSNWs have been studied. The top two rows are transverse plane TM modes with diameters varying from 20 nm to 370 nm at same wavelength (532 nm) of incident light. Bottom row is the longitudinal plane TM modes with length varying from  $0.5\mu m$  to  $3\mu m$  while remain the same diameters. The results demonstrated that with increasing of the diameters or lengths while remain the other factor same, the resonant mode numbers also increased correspondingly. However, if the diameter of the CSNW is smaller than 150 nm, there is no clear confined resonant modes excited by the structure which is consistent with the findings in

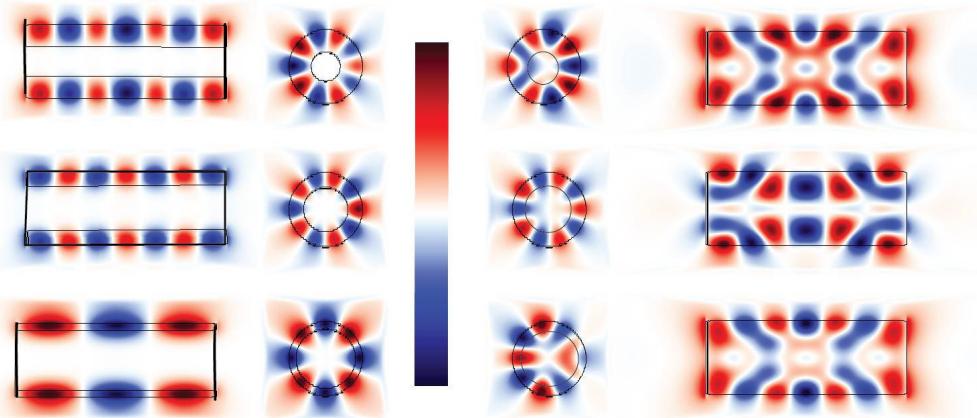


Figure 3.7 FDTD simulation results for different ratios, (top)  $r_{core} = 40\% r_{shell}$  (middle)  $r_{core} = 60\% r_{shell}$  and (bottom)  $r_{core} = 80\% r_{shell}$ , of core-shell radius of (left) air-core/AlGaAs-shell (right) GaAs-core/AlGaAs-shell cylindrical nanowires.

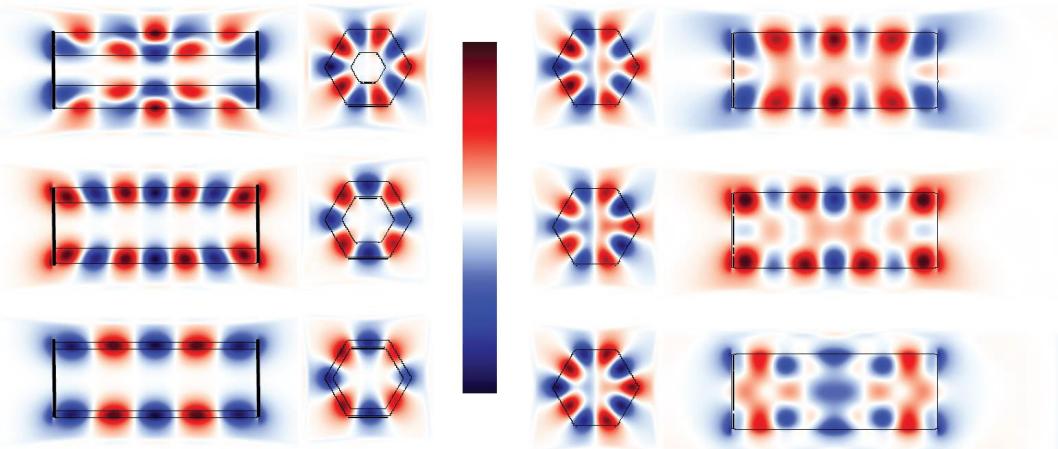


Figure 3.8 FDTD simulation results for different ratios, (top)  $r_{core} = 40\% r_{shell}$  (middle)  $r_{core} = 60\% r_{shell}$  and (bottom)  $r_{core} = 80\% r_{shell}$ , of core-shell radius of (left) air-core/AlGaAs-shell (right) GaAs-core/AlGaAs-shell hexagonal nanowires.

Ref. ??.

Additionally, figures 3.10(b) and 3.10(d) show simulation of cylindrical and hexagonal structures, respectively, with core of GaAs and shell of AlGaAs. These simulations show that there is little difference between core-only as in Fig. 3.10 (a, c) and core-shell (b, d) NWs, since the difference of the refractive indices of core and shell is small. Despite being optically identical, these structures have very different optoelectronic properties which will be discussed after describing the important ramifications of the optical analysis of NWs in Chapter 5.

### 3.2.4 Light Engineering of sub-wavelength Nano-structure

Dependence of the resonant modes on the cavity geometry offers an important degree of freedom to engineer a cavity for particular optical properties. Figure 3.11 shows the dependence of three volumetric TM resonant modes excitation wavelengths with radius. In this spectral range, only lower TM modes can be excited with smaller radii, e.g.,  $r = 40$  nm and 60 nm, however, as the radius increases, higher order modes can be excited, and the optical power corresponding to the lower order modes will be reduced. We observe redshift of these volumetric TM modes with increasing NW radius. Also, the wavelength variation of  $TM_{1n}$  mode is much larger compared to  $TM_{2n}$  and  $TM_{3n}$  modes. These observations demonstrate the feasibility to engineer the volumetric mode at certain wavelength, i.e., allow us to optimize absorption or emission at a desired frequency or certain incident optical power by controlling the radius and/or length of a NW thus providing the ability to engineer the absorption spectrum in order to match desired properties.

### 3.2.5 Tapering effect

The dependence of the resonant modes on NW radius also suggests the interesting possibility of having tapered structures which can support more than one resonant mode, thus be able to optimize the spectrum of interest. The metalorganic vapor phase epitaxy (MOVPE) or vapor liquid solid (VLS) growth methods are readily capable of forming nanowires with tapered sidewalls. The resultant cavity, however, does not support the superposition of the modes present in cylindrical

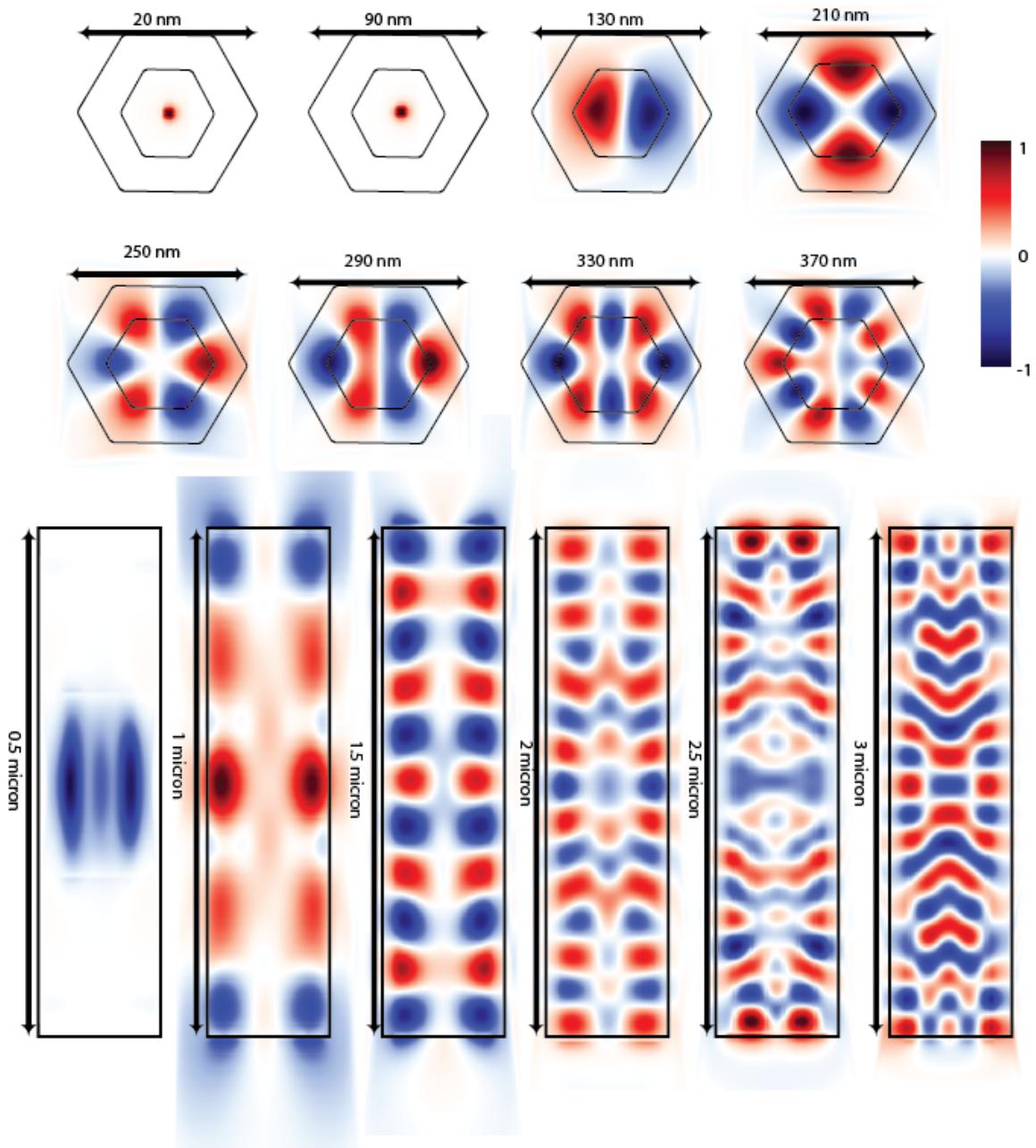


Figure 3.9 Geometric Dependence TM radius variation for different diameters and length. Top two rows are the transverse plane TM modes with diameters varying from 20 nm to 370 nm. Bottom row is the longitudinal plane TM modes with length varying from  $0.5\mu m$  to  $3\mu m$ .

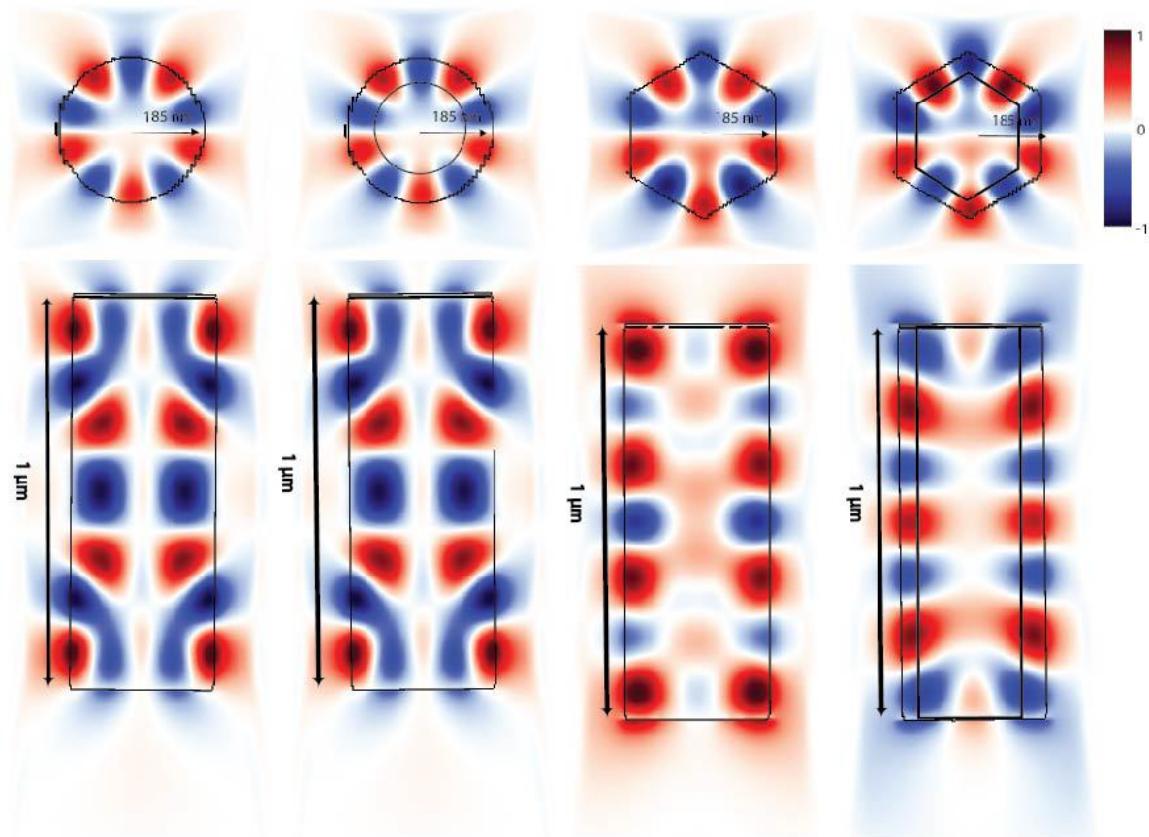


Figure 3.10 Cavity modes for (a) core-only cylindrical, (b) core-shell cylindrical, (c) hexagonal core-only, and (d) hexagonal core-shell. The radius of nanowire is 185 nm and the height is 1  $\mu m$ .

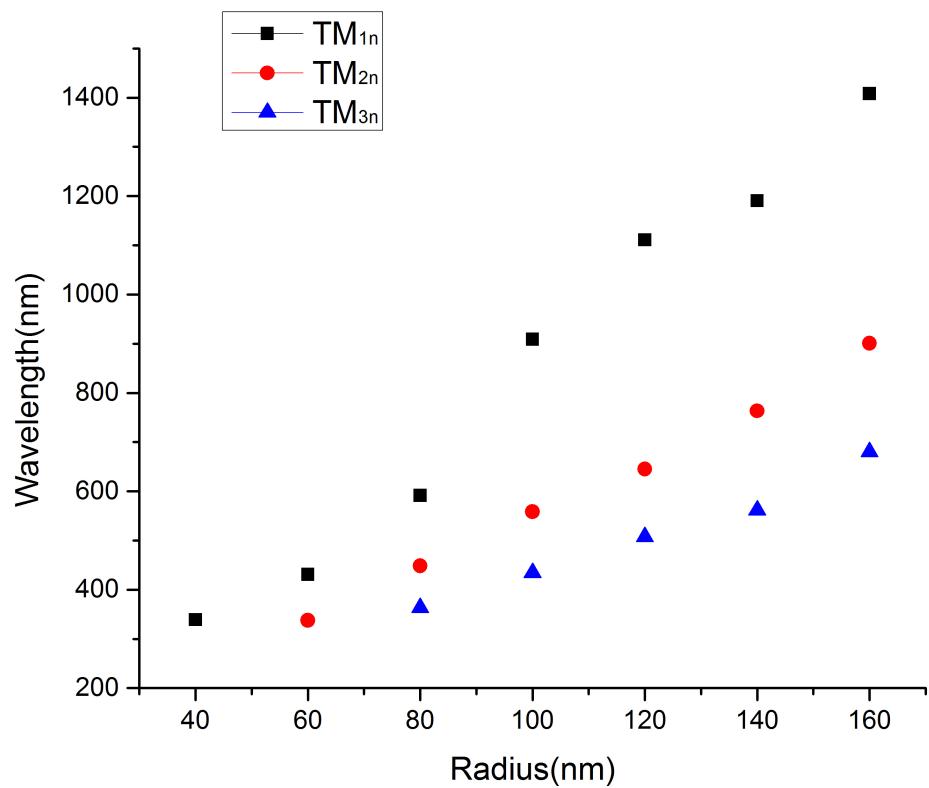


Figure 3.11 Correlation of the volumetric TM modes' excitation wavelength with NW radius allows optimization of cavity for absorption and emission at desired wavelengths.

structures of the same diameter; in fact tapered sidewalls have been identified as the primary loss mechanism for these sub-wavelength cavities.

The effect of tapering has been studied for hexagonal CSNW that were grown on a silicon substrate with average  $5^\circ$  angles between opposite sidewalls; vertical electrical field intensity ( $|E|^2$ ) profiles for (a)  $TM_{61}$  and (b)  $TM_{62}$  modes under different excitation wavelength are shown in Fig. 3.12, which similar to the result in Ref.<sup>2</sup>. Figure 3.12 (c, d) show first-order and higher-order transverse plane modes at different positions along the wire growth axis. The modes are primarily confined at the base, and become less resonant as they propagate upwards with decreasing of the radius at top. Higher-order axial modes generally have lower quality factor. Physically, the stronger Fabry-Perot characteristic of higher-order axial modes means that their effective longitudinal wave-vector components become stronger, causing larger penetration and loss into the substrate. Nevertheless, from a different perspective, multi-mode resonances can be achieved within certain wavelength range by controlling the tapering angle in order to form small varying radius along the nanostructure axial direction as in Fig. 3.12 (c, d). One can also red- or blue-shift the resonance peaks, since these volumetric resonance modes are dependent on transverse dimensions. Thus, intentioned tapering offers an alternative way to engineering the multi-mode resonances and finer tunability of these resonance peaks.

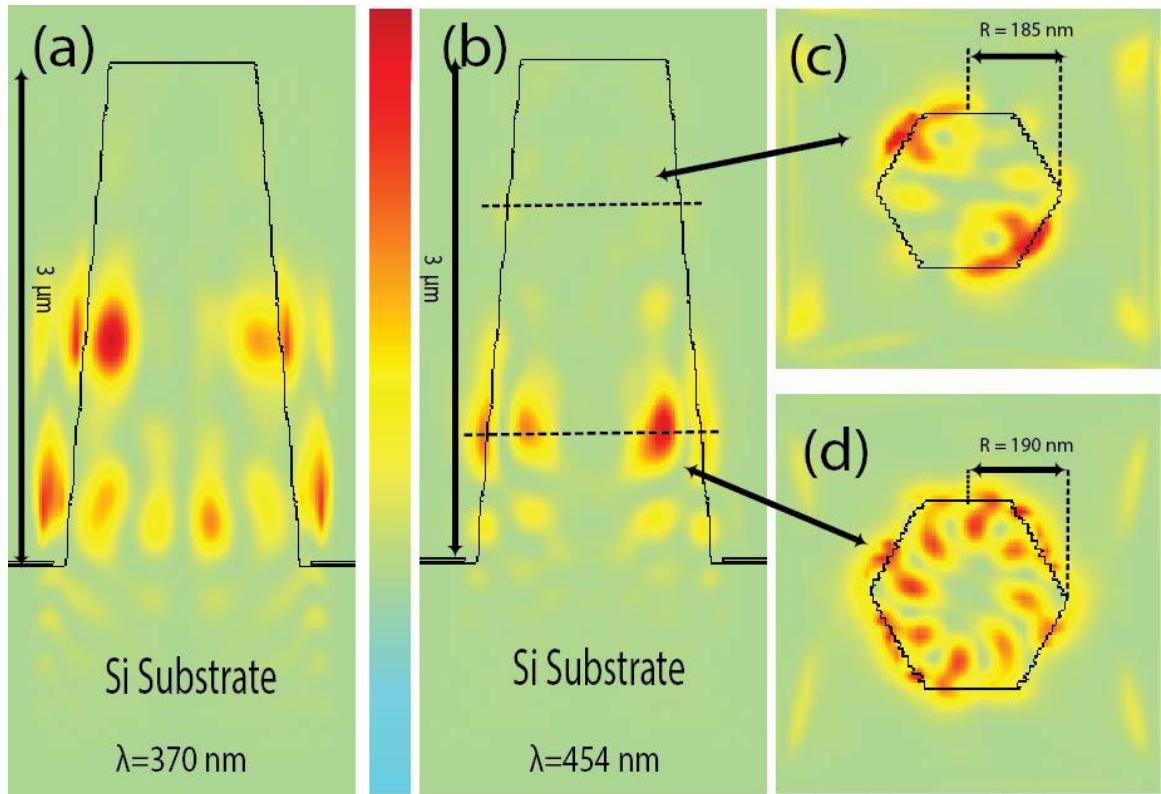


Figure 3.12 FDTD simulated electric field intensity distribution ( $|E|^2$ ) of hexagonal core-shell nanowire on top of Si substrate with 5° tapering effect. (a, b) field intensity distribution along axial direction with different incident light wavelength, (c, d) field intensity distribution in the transverse plane at different positions along the NW.

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## CHAPTER 4

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### REDUCED ELECTRONIC DENSITY DISTRIBUTION

A heterojunction is basically a p-n junction in a semiconductor between materials of different composition. Normal junctions are between p and n type versions of the same material. But in this case we refer to a junction formed between two group III-arsenide usually a GaAs/AlAs interface or a GaAs/AlGaAs interface. Since they are two different materials, the band structure is discontinuous from one material to the other and the band alignment across the interface is typically of type I, i.e. the band gap of the lower bandgap material is positioned energetically within the bandgap of the wider bandgap semiconductor.

Polarization fields The usual growth direction for hexagonal III-V materials is along the polar [0001] axis, for which the crystal lacks inversion symmetry. This will result in the formation of polarization fields. There are two kinds of polarization fields. They are spontaneous polarization (SP) and piezoelectric polarization (PZ). The spontaneous polarization exists in polar semiconductors with a Wurzite or lower symmetry crystal structure and is related to the deviation of the crystal lattice parameters from the ideal values for the structure, thereby creating molecular dipoles in the material building a polarization field just like that formed in ferroelectrics. This field has a fixed direction along the [0001] c-axis in the Wurtzite lattice. Therefore the field resulting from spontaneous polarization will point along the growth direction and this maximizes spontaneous polarization effect in these systems and renders the problem effectively one-dimensional.

The other type of polarization field, the piezoelectric polarization occurs due to the presence of strain in the system. When two layers are joined together to form a heterojunction, the difference in

the lattice constant between the two materials will lead to a strain . This strain also occurs due to the difference in the thermal expansion coefficients in the layers during cool down after growth. This leads to elastic strain in the layers.

## 4.1 Self-consistent Schrödinger-Poisson Solver

### 4.1.1 Finite Element Method

The study of energy band structures of heterostructures needs a detailed knowledge of optical and transport properties of the heterostructures. These properties can be found by solving self-consistently Poisson's and Schrödinger's equations for the electron wave functions.

The finite element method (FEM) is a simple and efficient method for solving ordinary differential equations (ODEs) or partial differential equations (PDEs) in problem regions with simple boundaries<sup>145</sup>. FEM can be used to solve for the Schrödinger and Poisson equation self-consistently. A generic formulation for a PDE with the following form:

$$|D|u(x) = f(x) \in \Omega \quad (4.1)$$

where  $D$  is an arbitrary operator, and  $\Omega$  defines the geometry. In order to solve this PDE using FEM, eq. 4.1 has to be rewritten in weak variational form with the boundary conditions:

$$\begin{cases} u(x) = u_0(x) & \text{on } \Gamma_D \\ \frac{\partial u}{\partial n} = g_0(x) & \text{on } \Gamma_N \end{cases} \quad (4.2)$$

where  $\Gamma_D$  and  $\Gamma_N$  signifies Dirichlet and Neumann boundary condition. By introducing an arbitrary function  $v$  and multiplying the PDE with  $v$ , then integrating over all the domain  $\Gamma$  and separating every second-order derivative using integration by parts, the original PDE can be carried out in the

weak form as:

$$\int_{\Omega} |D'|(\mathbf{u} \cdot \mathbf{v}) d\Omega + \int_{\Gamma_N} g v \partial\Omega = \int_{\Omega} f v d\Omega \quad \forall v \in \hat{V} \quad (4.3)$$

where  $D'$  is the reduced operator after performing integration by part to the second-order derivatives, and  $\hat{V}$  is the function space where an arbitrary function  $v$  belongs to. The function  $u$  lies in  $V$ , which could be different than  $\hat{V}$ . This continuous variational problem need to be reformulated to discrete problem with discrete space  $\hat{V}_d \subset \hat{V}$  and  $V \subset V$  so that the boundary conditions can be restated as:

$$\int_{\Omega} |D'|(\mathbf{u}_d \cdot \mathbf{v}) d\Omega + \int_{\Gamma_N} g v \partial\Omega = \int_{\Omega} f v d\Omega \quad \forall v \in \hat{V}_d \subset \hat{V} \quad (4.4)$$

It is more convenient to use unified notation for linear weak forms  $a(u, v) = L(v)$  with  $a(u, v) = \int_{\Omega} |D'|(\mathbf{u} \cdot \mathbf{v}) d\Omega$  and  $L(v) = \int_{\Omega} f v d\Omega - \int_{\Gamma_N} g v \partial\Omega$ .

#### 4.1.2 Variational form of Schrödinger and Poisson equations

A general Poisson equation for electrostatics is giving by<sup>146</sup>:

$$\frac{d}{dx} (\epsilon_s(x) \frac{d}{dx}) \Phi(x) = \frac{-q[N_D(x) - n(x)]}{\epsilon_0} \quad (4.5)$$

where  $\epsilon_s$  is the dielectric constant of the material,  $N_D$  is the ionized donor concentration,  $\Phi$  is electrostatic potential, and  $n$  is the electron density. Since Eq. 4.5 only has a piecewise dielectric constant, the domain can be divided into subdomains by different dielectric constants. The Poisson equation can be rewritten as:

$$\epsilon_s \nabla^2 \Phi(x) = \frac{-q[N_D(x) - n(x)]}{\epsilon_0} \quad (4.6)$$

Note that the operator  $|D|$  is replaced by  $\nabla^2$ , and the source term  $f(x)$  is replaced with the scaled difference of the ionized donor concentration and the electron density. Then the Poisson equation can be reformulate to the weak variational form following the previous procedures.

$$\int_{\Omega} \epsilon_s \epsilon_0 \nabla \Phi \nabla v \, d\Omega = \int_{\Omega} [-q[N_D(x) - n(x)]v(x) \, d\Omega] \quad (4.7)$$

The weak variational form of Schrödinger's equation can be derived from the general differential form following by the similar manner:

$$-\frac{\hbar^2}{2} \frac{d}{dx} \left( \frac{1}{m^*(x)} \frac{d}{dx} \right) \psi(x) + V(x)\psi(x) = E\psi(x) \quad (4.8)$$

where  $m^*(x)$  is the effective mass. Equation 4.8 can rewritten after taking the effective mass out, as it will remain constant in a single region.

$$\frac{\hbar^2}{2m^*} \nabla^2 \psi(x) + [E - V(x)]\psi(x) = 0 \quad (4.9)$$

Multiply both sides by a test function  $v$ , which is arbitrary with the condition that it vanishes on the boundaries of the system.

$$\int_{\Omega} \frac{\hbar^2}{2m^*} \frac{\psi}{x} \frac{v}{x} \, d\Omega + \int_{\Omega} V(x)\psi(x)v(x) \, d\Omega = \int_{\Omega} E\psi(x)v(x) \, d\Omega \quad (4.10)$$

#### 4.1.3 Numerical Implementation

To obtain the electronic properties, the electrostatic potential  $V(x = -q\phi(x) + \Delta E_c(x))$  first sets to zero. Then the envelope functions and the eigen energies are calculated according to the Schrödinger equation 4.8. A Poisson equation 4.5 is solved after the determination of the quasi Fermi level  $E_F$

by solving charge neutrality equation. The electron concentration can now be calculated based on:

$$n(x) = \sum_{k=1}^m \psi_k^*(x) \psi_k(x) n_k \quad (4.11)$$

$$n_k = \frac{m^*}{\pi \hbar^2} \int_{E_k}^{\infty} \frac{1}{1 + e^{(E - E_F)/KT}} dE \quad (4.12)$$

where  $\Delta E_c(x)$  is the pseudopotential energy due to the band offset at the heterointerface,  $n_k$  is the electron occupation number which can be calculated by Fermi-Dirac distribution function with Fermi level  $E_F$ ,  $\psi_k$  is the wavefunction in the  $k^{th}$  state, and  $E_k$  is the eigen energy in state k. Finally, a check of the electrostatic potential update decides whether the iteration terminates. The procedure of this Schrödinger-Poisson solver has been demonstrated in the flow chart diagram as in Fig. 4.1.

Implementing the FEM method when solving the Schrödinger and Poisson equations requires the construction of a mesh defining local coordinate surfaces. For each node of this mesh, the unknown eigen functions and eigen values are found, replacing the original differential equations by variational forms. In order to make the FEM method more effective, implementing a small mesh when the wavefunction is changing rapidly and a large mesh during a slow change in the wavefunction is necessary.

## 4.2 Electronic Distribution in Nanowires

The electronic band structure and the electronic density of cylindrical and hexagonal GaAs/Al-GaAs core-shell nanowire are calculated self-consistently by solving Poisson and Schrödinger equations<sup>147,148</sup> using **nextnano<sup>3</sup>** simulation packages<sup>149</sup>, which is a commercial computer aid software with better physical method for the calculation of the quantum mechanical properties of an arbitrary combination of geometries and materials.

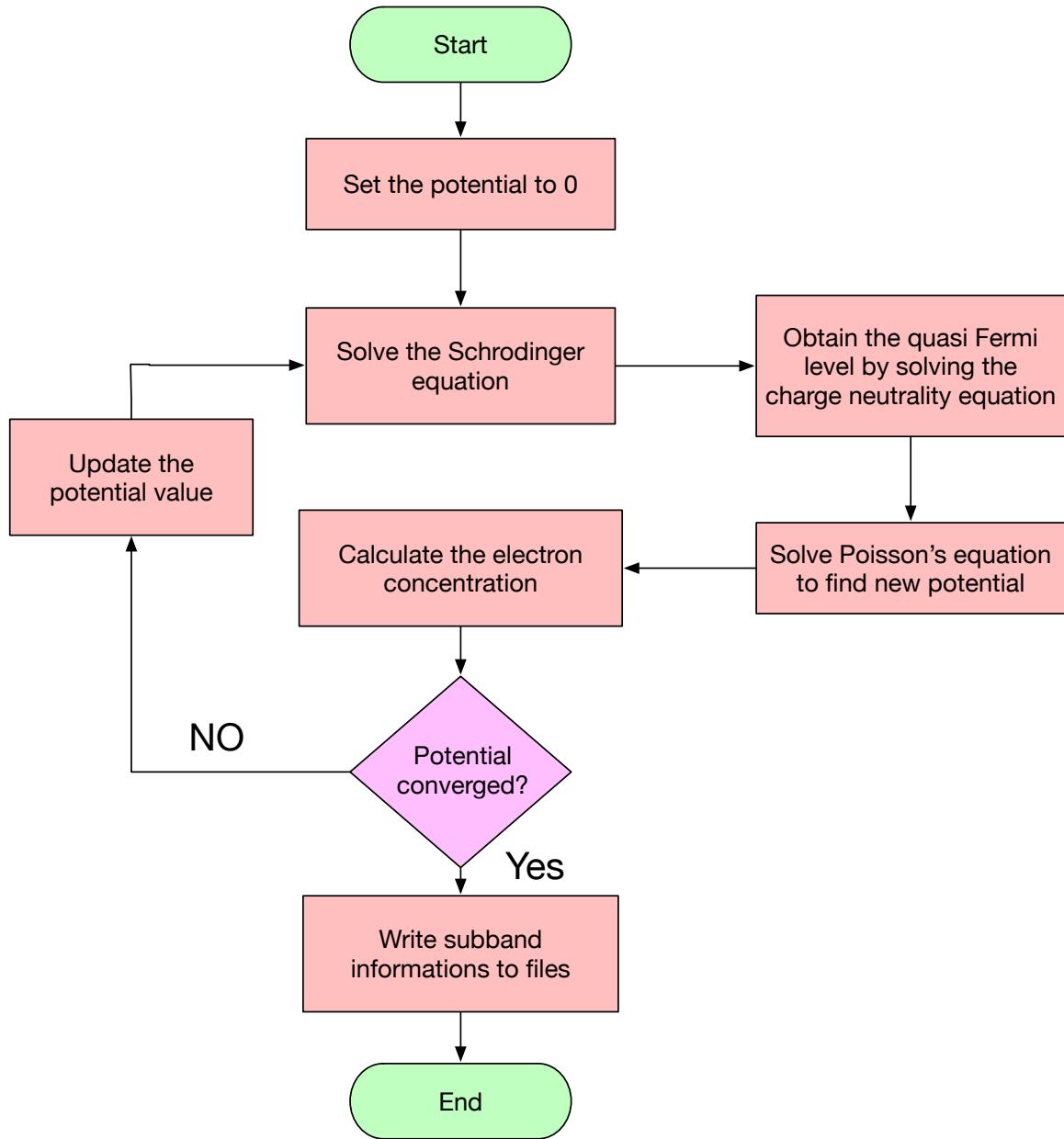


Figure 4.1 A flow chart diagram of the Schrödinger-Poisson solver. The procedure is only discussed for electrons in the conduction band for simplicity but it also hold true for holes in the valence band using analogous formulas.

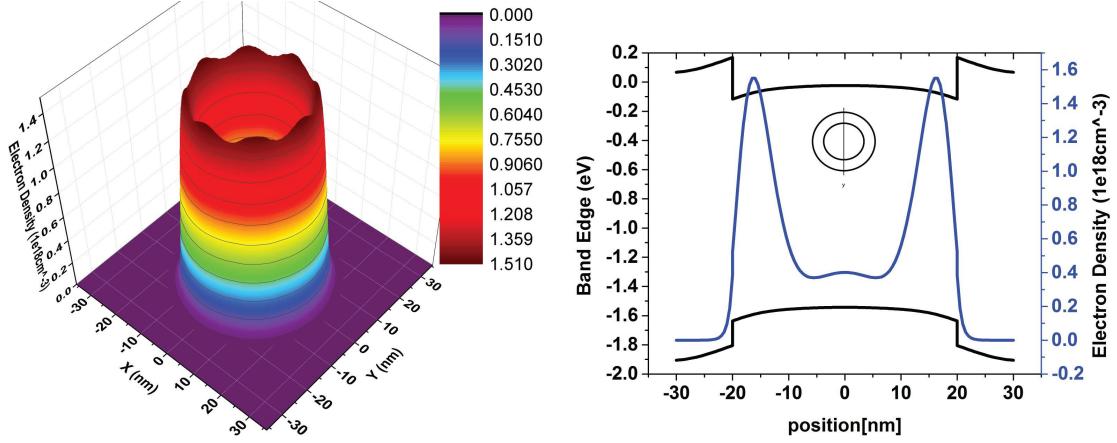


Figure 4.2 (left) Electron charge distribution in 3D illustration. (right) Conduction and valence band bending (black lines) and electron density distribution (blue line) for cylindrical core-shell nanowire. The inset shows the data captured from a vertical slice of the simulated structure.

#### 4.2.1 Cylindrical Core-Shell Nanowire

The cylindrical core-shell nanowire has been investigated with a radius of 20nm GaAs core and 15nm AlGaAs shell. An additional Si-doped AlGaAs layer with a 0.33 mole fraction is placed between the core and shell. The thickness of this layers is 5 nm. The left part of Fig. 4.2 shows the electron density distribution in 3D view. A free-electron gas is formed in the GaAs core and at the inner heterointerface with a small fluctuation of density along the interface. There is a very small amount of electron gas distributed at the center of the core. Further simulation with different doping density  $\rho_D$  shows similar distribution of the electron gas but very small variation of the magnitude of the intensity. On the right part of Fig. 4.2, the black line represents the conduction and valence band bending and the blue line shows the electron density along the vertical cut of this cylindrical CSNW.

#### 4.2.2 Hexagonal Core-shell Nanowire

Due to the hetero-interface between the core and shell and the piezoelectric force at the corners, the electronic states distribution inside of the hexagonal core-shell nanowire is not always three-dimensional case or two-dimensional like in cylindrical NWs. Lower-dimensional electron gas arises with increased doping density. A delta-doped hexagonal CSNW heterostructure has been simulated.

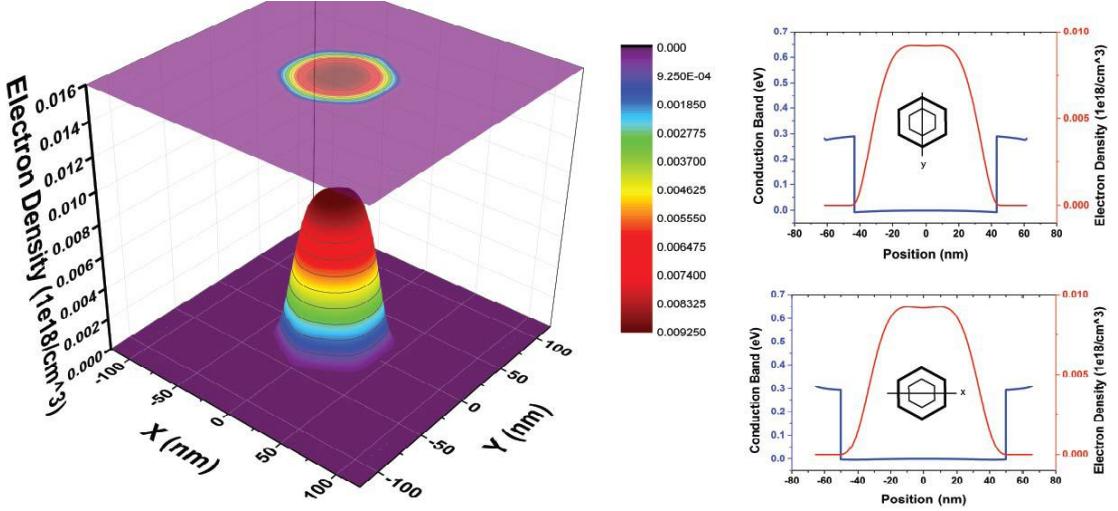


Figure 4.3 (left) Three dimensional electron charge distribution in 3D illustration. (right) Conduction and valence band bending (blue lines) and electron density distribution (red line) for hexagonal core-shell nanowire with a low doping density. The inset shows the data captured from a (top) vertical or (bottom) horizontal slice of the simulated structure.

The radius of GaAs core and AlGaAs shell is 43.3 nm and 45 nm, respectively, with a 17.3 nm AlGaAs spacer in between. The thickness of Si-doped AlGaAs is 1.6 nm with a 0.33 mole fraction of AlGaAs. This Si-doped AlGaAs layer is used to populate a (triangular) quantum well at the heterointerfaces. Such a well can also be produced by sandwiching a GaAs layer radially between two wider bandgap materials.

The left part of Fig. 4.3, 4.4 and 4.5 shows the spatial distribution of the free-electron gas for the three values of the doping density indicated as (Fig. 4.3)  $\rho_D = 9.2 \times 10^{18} \text{ cm}^{-3}$ , (Fig. 4.4)  $\rho_D = 9.6 \times 10^{18} \text{ cm}^{-3}$ , (Fig. 4.3)  $\rho_D = 1.5 \times 10^{19} \text{ cm}^{-3}$ . On the right part, the electronic band structure (blue line) and the electronic density (red line) of hexagonal GaAs/AlGaAs core-shell nanowire are depicted for vertical slice (top, right) or horizontal slice (bottom, right).

At the lowest doping, shown in Fig. 4.3, the charge is distributed deep into the core. The distribution is only slightly modulated (right panels) crossing the core along either the y cross section or x cross section, and slightly depleted in the center of the core.

As the doping is increased in Fig. 4.4, the charge depletion in the center is more pronounced, and the

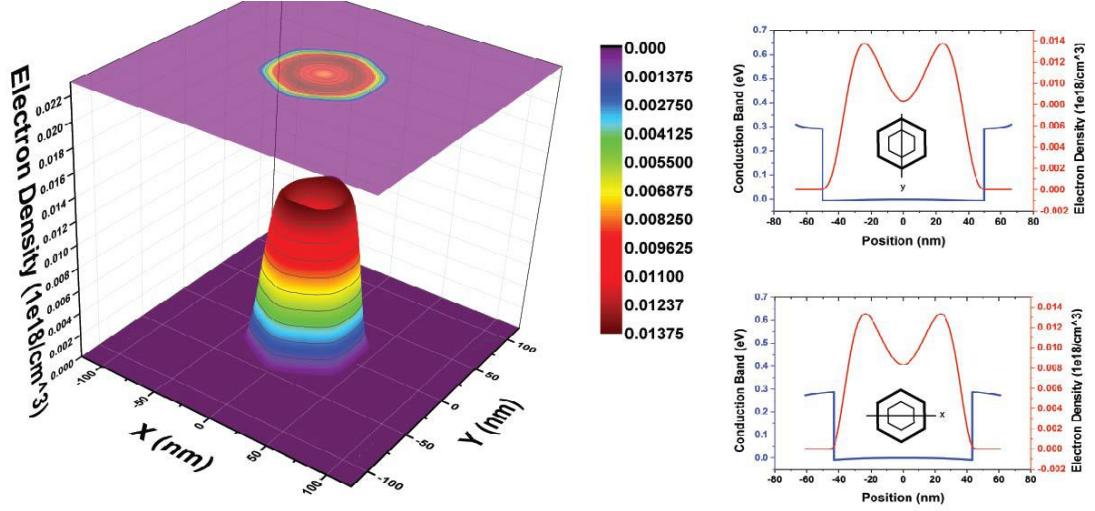


Figure 4.4 (left) Two dimensional electron charge distribution in 3D illustration. (right) Conduction and valence band bending (blue lines) and electron density distribution (red line) for hexagonal core-shell nanowire with a moderate doping density. The inset shows the data captured from a (top) vertical or (bottom) horizontal slice of the simulated structure.

charge moves toward the heterojunction interface, leaving this "volcano" like charge distribution in the left part of Fig. 4.4. The two-dimensional electron gases (2DEG) are formed at the heterointerface of GaAs core and AlGaAs shell.

As the doping is further increased in Fig. 4.5, the shell 2DEG form at the six (6) core-shell heterointerface facets, with six (6) pillars of one-dimensional electron gas (1DEG) forming at the 6 vortices. In addition, as shown in the right part of the Fig. 4.3, 4.4 and 4.5, the electronic density of Fig. 4.5 is around two orders of magnitude higher than 2DEG and bulk counterparts. The results also matched the other groups' simulation results very well<sup>147,148</sup>.

### 4.3 Conclusions

In this chapter, the finite-element-method implemented self-consistent Shrödinger-Poisson solver has been discussed. In addition, a cylindrical and hexagonal core-shell nanowire structure has been simulated and compared with different doping density. The simulated results show unique electron density distribution in hexagonal CSNW with large doping density. This unique distribution of

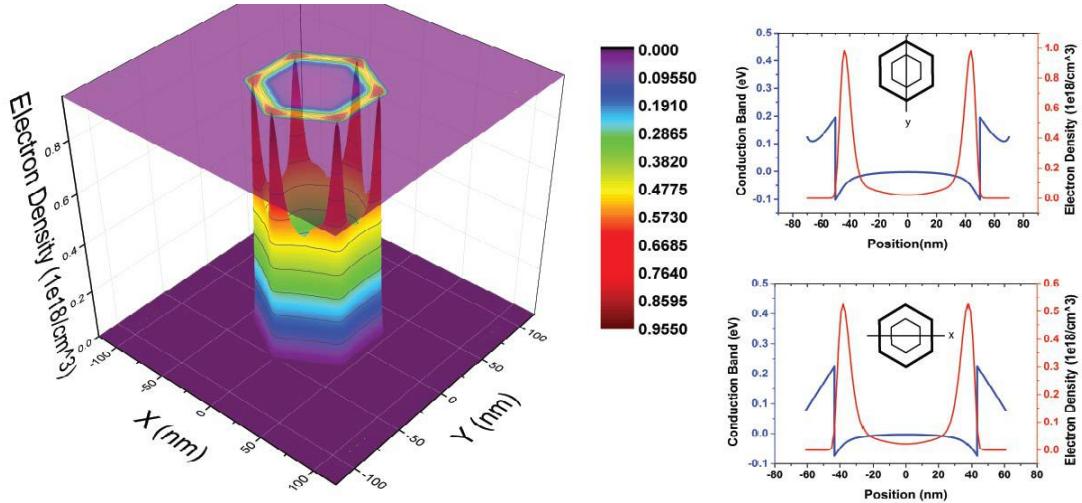


Figure 4.5 (left) One dimensional electron charge distribution in 3D illustration. (right) Conduction and valence band bending (blue lines) and electron density distribution (red line) for hexagonal core-shell nanowire with a high doping density. The inset shows the data captured from a (top) vertical or (bottom) horizontal slice of the simulated structure.

electrons has also been verified experimentally by electron holographic tomography<sup>150</sup>

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## CHAPTER 5

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### DIMENSIONAL DEPENDENCE OF OPTICAL TRANSITION RATES

#### 5.0.1 Fermi's Golden Rule

When the semiconductor illuminated by light, the interaction between the photons and the electrons in the semiconductor can be described by the Hamiltonian:

$$\mathcal{H} = \frac{1}{2m_0}(\mathbf{p} - e\mathbf{A})^2 + V(\mathbf{r}) \quad (5.1)$$

where  $m_0$  is the free electron mass,  $e = -|e|$  for electrons,  $\mathbf{A}$  is the vector potential accounting for the presence of the electromagnetic field, and  $V(\mathbf{r})$  is the periodic crystal potential.

The Hamiltonian can be expanded into

$$\mathcal{H} = \frac{1}{2m_0}(\mathbf{p} - e\mathbf{A})^2 + V(\mathbf{r}) \approx \mathcal{H}_0 + \mathcal{H}' \quad (5.2)$$

where  $\mathcal{H}_0$  is the unperturbed Hamiltonian and  $\mathcal{H}'$  is considered as a perturbation due to light

$$\mathcal{H}_0 = \frac{\mathbf{p}^2}{2m_0} + V(\mathbf{r}) \quad (5.3)$$

$$\mathcal{H}' = -\frac{e}{m_0} \mathbf{A} \cdot \mathbf{p} \quad (5.4)$$

and consider the coulomb gauge has been used.

$$\nabla \cdot \mathbf{A} = 0 \quad (5.5)$$

noting that  $\mathbf{p} = (\hbar/i)\nabla$ , so  $\mathbf{p} \cdot \mathbf{A} = (\frac{\hbar}{i})\nabla \cdot \mathbf{A} = \mathbf{A} \cdot \mathbf{p}$ . And since we know  $\mathbf{p} \approx \hbar k \approx \hbar \frac{\pi}{a}$ , and  $a$  is the lattice constant, usually have a value of  $5\text{\AA}$ , so  $|e\mathbf{A}| \ll |\mathbf{p}|$ , then we can drop the last term  $\frac{e^2 \mathbf{A}^2}{2m_0}$ , because it is much smaller than the terms linear in  $\mathbf{A}$ .

Assume the vector potential for the optical electric field of the form

$$\mathbf{A} = \hat{e} \mathbf{A}_0 \cos k_{op} \cdot \mathbf{r} - \omega t = \hat{e} \frac{A_0}{2} e^{ik_{op} \cdot \mathbf{r}} e^{-i\omega t} + \hat{e} \frac{A_0}{2} e^{-ik_{op} \cdot \mathbf{r}} e^{i\omega t} \quad (5.6)$$

where  $\mathbf{k}_{op}$  is the wave vector,  $\omega$  is the optical angular frequency, and  $\hat{e}$  is a unit vector in the direction of the optical electric field, we have

$$\mathbf{E}(\mathbf{r}, t) = -\frac{\partial \mathbf{A}}{\partial t} = -\hat{e}\omega A_0 \sin \mathbf{k}_{op} \cdot \mathbf{r} - \omega t \quad (5.7)$$

$$\mathbf{H}(\mathbf{r}, t) = \frac{1}{\mu} \nabla \times \mathbf{A} = -\frac{1}{\mu} \mathbf{k}_{op} \times \hat{e} A_0 \sin(\mathbf{k}_{op} \cdot \mathbf{r} - \omega t) \quad (5.8)$$

where we have used the fact that the scalar potential  $\varphi$  vanishes ( $\rho = 0$ ) for the optical field, and  $\mu = \mu_0$ , the permeability of the free space. The Poynting vector for the power intensity ( $\text{W/cm}^2$ ) is

given by

$$\mathbf{P}(\mathbf{r}, t) = \mathbf{E}(\mathbf{r}, t) \times \mathbf{H}(\mathbf{r}, t) = \hat{k} \mathbf{k}_{\text{op}} \frac{\omega A_0^2}{\mu} (\mathbf{k}_{\text{op}} \cdot \mathbf{r} - \omega t) \quad (5.9)$$

which is pointing along the direction of wave propagation  $\mathbf{k}_{\text{op}}$ . The time average of the Poynting flux is simply

$$\begin{aligned} \mathbf{P} &= |\mathbf{P}(\mathbf{r}, t)| = \frac{\omega A_0^2}{2\mu} \mathbf{k}_{\text{op}} \\ &= \frac{\omega^2 A_0^2 n_r}{2\mu c} \\ &= \frac{\omega^2 A_0^2 n_r \sqrt{\mu_0 \epsilon_0}}{2\mu_0} \\ &= \frac{\omega^2 A_0^2 n_r \sqrt{\epsilon_0}}{2\sqrt{\mu_0}} \\ &= \frac{\omega^2 A_0^2 n_r \sqrt{\epsilon_0} \sqrt{\epsilon_0}}{2\sqrt{\mu_0} \sqrt{\epsilon_0}} \\ &= \frac{\omega^2 A_0^2 n_r \epsilon_0 c}{2} \end{aligned} \quad (5.10)$$

Noting the time average of the  $\sin^2()$  function is  $\frac{1}{2}$  and  $\mathbf{k}_{\text{op}} = \omega \sqrt{\mu \epsilon_0} = \frac{\omega}{v} = \frac{\omega}{c/n_r}$ ,  $c = \frac{1}{\sqrt{\mu_0 \epsilon_0}}$

The interaction Hamiltonian

$$\begin{aligned} \mathcal{H}'(\mathbf{r}, t) &= -\frac{e}{m_0} \mathbf{A}(\mathbf{r}, t) \cdot \mathbf{p} \\ &= \mathcal{H}'(\mathbf{r}) e^{-i\omega t} + \mathcal{H}'^+(\mathbf{r}) e^{+i\omega t} \end{aligned} \quad (5.11)$$

where

$$\mathcal{H}'(\mathbf{r}) = -\frac{e A_0 e^{i\mathbf{k}_{\text{op}} \cdot \mathbf{r}}}{2m_0} \cdot \hat{\mathbf{e}} \cdot \mathbf{p} \quad (5.12)$$

The superscript “+” means the Hermitian adjoint operator.

The transition rate for the absorption of a photon:

If the electron is at state a initially. And assume  $E_b > E_a$

$$W_{\text{abs}} = \frac{2\pi}{\hbar} \left| \langle b | \mathcal{H}'(\mathbf{r}) | a \rangle \right|^2 \delta(E_b - E_a - \hbar\omega) \quad (5.13)$$

The total upward transition rate per unit volume ( $s^{-1}\text{cm}^{-3}$ ) in the crystal taking into account the probability that state a is occupied and state b is empty:

$$R_{a \rightarrow b} = \frac{2}{V} \sum_{\mathbf{k}_a} \sum_{\mathbf{k}_b} \frac{2\pi}{\hbar} \left| \mathcal{H}'_{ba} \right|^2 \delta(E_b - E_a - \hbar\omega) f_a (1 - f_b) \quad (5.14)$$

where we sum over the initial and final states and assume that the Fermi-Dirac distribution  $f_a$  is the probability that the state a is occupied. A similar expression holds for  $f_b$  with  $E_a$  replaced by  $E_b$ , and  $(1 - f_b)$  is the probability that the state b is empty. The prefactor 2 takes into account the sum over spins, and the matrix element  $\mathcal{H}'_{ba}$  is given by **Fermi's Golden Rule**

$$\mathcal{H}'_{ba} \equiv \left| \langle b | \mathcal{H}'(\mathbf{r}) | a \rangle \right| = \int \Psi_b^*(\mathbf{r}) H'(\mathbf{r}, t) \Psi_a(\mathbf{r}) d^3r \quad (5.15)$$

Similarly, the transition rate for the emission of a photon if an electron is initially at state b is

$$W_{\text{ems}} = \frac{2\pi}{\hbar} \left| \langle a | \mathcal{H}'(\mathbf{r}) | b \rangle \right|^2 \delta(E_a - E_b + \hbar\omega) \quad (5.16)$$

The downward transition rate per unit volume ( $s^{-1}\text{cm}^{-3}$ ) is

$$R_{b \rightarrow a} = \frac{2}{V} \sum_{\mathbf{k}_a} \sum_{\mathbf{k}_b} \frac{2\pi}{\hbar} \left| \mathcal{H}'^{+}_{ab} \right|^2 \delta(E_a - E_b + \hbar\omega) f_b (1 - f_a) \quad (5.17)$$

Using the even property of the delta function,  $\delta(-x) = \delta(x)$ , and  $\mathcal{H}'_{ba} = \mathcal{H}'^{+}_{ab}$ , the net upward

transition rate per unit volume can be written as

$$R = R_{a \rightarrow b} - R_{b \rightarrow a} = \frac{2}{V} \sum_{\mathbf{k}_a} \sum_{\mathbf{k}_b} \frac{2\pi}{\hbar} \left| \mathcal{H}'_{ba} \right|^2 \delta(E_b - E_a - \hbar\omega) (f_a - f_b) \quad (5.18)$$

The absorption coefficient  $\alpha(1/cm)$  in the crystal is the fraction of photons absorbed per unit distance:

$$\alpha = \frac{\text{Number of photons absorbed per second per unit volume}}{\text{Number of injected photons per second per unit area}} \quad (5.19)$$

The injected number of photons per second per unit area is the optical intensity  $P(W/cm^2)$  divided by the energy of a photon  $\hbar\omega$ :

$$\alpha(\hbar\omega) = \frac{R}{\frac{P}{\hbar\omega}} = \frac{\hbar\omega}{\left(\frac{n_r c \epsilon_0 \omega^2 A_0^2}{2}\right)} R \quad (5.20)$$

Using the long wavelength approximation that  $\mathbf{A}(\mathbf{r}) = \mathbf{A}e^{i\mathbf{k}_{\text{op}} \cdot \mathbf{r}} \approx \mathbf{A}$ , we find that the matrix element can be written in terms of the momentum matrix element

$$\mathcal{H}'_{ba} = -\frac{e}{m_0} \mathbf{A} \cdot \langle b | \mathbf{p} | a \rangle = \frac{eA_0}{2m_0} \cdot \hat{\mathbf{e}} \cdot \mathbf{p}_{ba} \quad (5.21)$$

The absorption coefficient becomes

$$\begin{aligned} \alpha(\hbar\omega) &= C_0 \frac{2}{V} \sum_{\mathbf{k}_a} \sum_{\mathbf{k}_b} |\hat{\mathbf{e}} \cdot \mathbf{p}_{ba}|^2 \delta(E_b - E_a - \hbar\omega) (f_a - f_b) \\ C_0 &= \frac{\pi e^2}{n_r \epsilon_0 c m_0^2 \omega} \end{aligned} \quad (5.22)$$

## 5.1 Interband Absorption for a Bulk Semiconductor

Evaluate the optical matrix element:

$$\mathcal{H}'_{ba} = \left\langle b \left| -\frac{e\mathbf{A}(\mathbf{r})}{m_0} \cdot \mathbf{p} \right| a \right\rangle \quad (5.23)$$

The vector potential for the optical field is

$$\mathbf{A}(\mathbf{r}) = \mathbf{A} \cdot e^{i\mathbf{k}_{op} \cdot \mathbf{r}} = \frac{\hat{e}A_0}{2} e^{i\mathbf{k}_{op} \cdot \mathbf{r}} \quad (5.24)$$

The Bloch functions for electrons in the valence band  $E_a$  and the conduction band  $E_b$  are:

$$\Psi_a(\mathbf{r}) = u_v(\mathbf{r}) \frac{e^{i\mathbf{k}_v \cdot \mathbf{r}}}{\sqrt{V}} \quad (5.25)$$

$$\Psi_b(\mathbf{r}) = u_c(\mathbf{r}) \frac{e^{i\mathbf{k}_c \cdot \mathbf{r}}}{\sqrt{V}} \quad (5.26)$$

where  $u_v(\mathbf{r})$  and  $u_c(\mathbf{r})$  are the periodic parts of the Bloch functions, and the remainders are the envelope functions (plane waves) for a free electron. The momentum matrix element is derived from

$$\begin{aligned} \mathcal{H}'_{ba} &= -\frac{eA_0}{2m_0} \hat{e} \cdot \int \Psi_b^* e^{i\mathbf{k}_{op} \cdot \mathbf{r}} \mathbf{p} \Psi_a d^3 r \\ &= -\frac{eA_0}{2m_0} \hat{e} \cdot \int u_c(\mathbf{r}) e^{i\mathbf{k}_c \cdot \mathbf{r}} e^{i\mathbf{k}_{op} \cdot \mathbf{r}} \left[ \left( \frac{\hbar}{i} \nabla u_v(\mathbf{r}) \right) e^{i\mathbf{k}_v \cdot \mathbf{r}} + \hbar \mathbf{k}_v u_v(\mathbf{r}) e^{i\mathbf{k}_v \cdot \mathbf{r}} \right] \frac{d^3 r}{V} \\ &\approx -\frac{eA_0}{2m_0} \hat{e} \cdot \int_{\Omega} u_c^*(\mathbf{r}) \frac{\hbar}{i} \nabla u_v(\mathbf{r}) \frac{d^3 r}{V} \int_V e^{i(-\mathbf{k}_c + \mathbf{k}_{op} + \mathbf{k}_v) \cdot \mathbf{r}} \frac{d^3 r}{V} \\ &= -\frac{eA_0}{2m_0} \hat{e} \cdot \mathbf{p}_{cv} \delta_{\mathbf{k}_c, \mathbf{k}_{op} + \mathbf{k}_v} \end{aligned} \quad (5.27)$$

$$\mathbf{p}_{cv} = \int_{\Omega} u_c^*(\mathbf{r}) \frac{\hbar}{i} \nabla u_v(\mathbf{r}) \frac{d^3 r}{\Omega} \quad (5.28)$$

where we noted that  $[u_c^*(\mathbf{r}) \frac{\hbar}{i} \nabla u_v(\mathbf{r})]$  and  $[u_c^*(\mathbf{r}) u_v(\mathbf{r})]$  are periodic functions with the period of a unit cell, whereas the envelope functions are slowly varying functions over a unit cell. Therefore, the integral over  $d^3 \mathbf{r}$  can be separated into the product of two integrals, one over the unit cell  $\Omega$  for the periodic part, and the other over the slowly varying part. In another word, we use the approximation:

$$\int_V \left[ u_c^*(\mathbf{r}) \frac{\hbar}{i} \nabla u_v(\mathbf{r}) \right] F(\mathbf{r}) d^3 \mathbf{r} \approx \int_V F(\mathbf{r}) d^3 \mathbf{r} \int_{\Omega} u_c^*(\mathbf{r}) \frac{\hbar}{i} \nabla u_v(\mathbf{r}) \frac{d^3 \mathbf{r}}{\Omega} \quad (5.29)$$

where  $F(\mathbf{r})$  is slowly varying over a unit cell, and we have used the periodic property of the Bloch periodic functions

$$u_c^*(\mathbf{r}) \frac{\hbar}{i} \nabla u_v(\mathbf{r}) = \sum_{\mathbf{G}} C_{\mathbf{G}} e^{i \mathbf{G} \cdot \mathbf{r}} \quad (5.30)$$

where the vectors  $\mathbf{G}'s$  are the reciprocal lattice vectors. Because  $F(\mathbf{r})$  is slowly varying over a unit cell, we may approximate  $F(\mathbf{r} + \mathbf{R}) = F(\mathbf{R})$  and put it outside of the integral over a unit cell. Here the  $\mathbf{R}s$  are the lattice vectors, and  $e^{i \mathbf{G} \cdot \mathbf{R}} = 1/\omega$  is the volume of a unit cell. Note that the orthogonal property

$$\begin{aligned} \int_{\Omega} u_c^* u_v d^3 \mathbf{r} &= 0, \\ \frac{1}{\Omega} \int_{\Omega} u_c^* u_c d^3 \mathbf{r} &= \frac{1}{\Omega} \int_{\Omega} u_v^* u_v d^3 \mathbf{r} = 1 \end{aligned} \quad (5.31)$$

From the matrix element, we see the momentum conservation

$$\hbar\mathbf{k}_c = \hbar\mathbf{k}_v + \hbar\mathbf{k}_{\text{op}} \quad (5.32)$$

is obeyed. The electron at the final state has its crystal momentum  $\hbar\mathbf{k}_c$  equal to its initial momentum  $\hbar\mathbf{k}_v$  plus the photon momentum  $\hbar\mathbf{k}_{\text{op}}$ . Because  $\mathbf{k}_{\text{op}} \sim \frac{2\pi}{\lambda_0}$ , and the magnitudes  $\mathbf{k}_c, \mathbf{k}_v$  are of the order  $\frac{2\pi}{a_0}$ , where  $a_0$  is the lattice constant of the semiconductors, which is typically of the order  $5.5\text{\AA}$  and is much smaller than we may ignore  $\mathbf{k}_{\text{op}}$  and obtain

$$\mathcal{H}'_{\text{ba}} \approx -\frac{eA_0}{2m_0} \hat{\mathbf{e}} \cdot \mathbf{p}_{\text{cv}} \delta_{\mathbf{k}_c, \mathbf{k}_v} \quad (5.33)$$

which is the **K-selection Rule**.

- 1) Interband momentum matrix element  $\mathbf{p}_{\text{cv}}$  depend only on the periodic parts of the Bloch functions ( $u_c$  and  $u_v$ ),
- 2) The original optical momentum matrix element  $\mathbf{p}_{\text{ab}}$ , depends on the full wave functions (i.e. including the envelope function).

Using the **K-selection rule** in the matrix element, we find that the absorption coefficient for a bulk semiconductor is

$$\alpha(\hbar\omega) = C_0 \frac{2}{V} \sum_{\mathbf{k}_a} \sum_{\mathbf{k}_b} |\hat{\mathbf{e}} \cdot \mathbf{p}_{\text{cv}}|^2 \delta(E_c - E_v - \hbar\omega)(f_v - f_c)$$

$$C_0 = \frac{\pi e^2}{n_r \epsilon_0 c m_0^2 \omega} \quad (5.34)$$

where the Fermi-Dirac distributions for the electrons in the valence bend and in the conduction band

are, respectively.

$$f_v(k) = \frac{1}{1 + e^{\frac{(E_v(k) - F_v)}{kT}}}, f_c(k) = \frac{1}{1 + e^{\frac{(E_c(k) - F_c)}{kT}}} \quad (5.35)$$

Assume:

- 1)  $\mathbf{k}_c = \mathbf{k}_v = \mathbf{k}$ ,  $F_v = F_c = E_F$  (thermal equilibrium)
- 2)  $f_v = 1$  and  $f_c = 0$
- 3)  $|\hat{e} \cdot \mathbf{p}_{cv}|^2$  is independent of  $\mathbf{k}$  and denote the absorption spectrum at thermal equilibrium.

$$\alpha(\hbar\omega) = C_0 |\hat{e} \cdot \mathbf{p}_{cv}|^2 \int \frac{2d^3k}{(2\pi)^3} \delta(E_g + \frac{\hbar^2 \mathbf{k}^2}{2m_r^*} - \hbar\omega) \quad (5.36)$$

where used the reduced effective mass  $m_r^*$

$$\begin{aligned} E_c &= E_g + \frac{\hbar^2 \mathbf{k}^2}{2m_r^*} & E_v &= -\frac{\hbar^2 \mathbf{k}^2}{2m_r^*} \\ \frac{1}{m_r^*} &= \frac{1}{m_e^*} + \frac{1}{m_h^*} \end{aligned}$$

Here all energies are measured from the top of the valence band. Therefore, both  $E_c$  and  $F_c$  contain the band-gap energy  $E_g$ . Let

$$X = E_g + E - \hbar\omega \quad E = \frac{\hbar^2 \mathbf{k}^2}{2m_r^*} \quad (5.37)$$

we find, by a change of variables, the integration can be carried out with the contribution at  $X = 0$ , and  $E = \hbar\omega - E_g$

$$\alpha(\hbar\omega) = C_0 |\hat{e} \cdot \mathbf{p}_{cv}|^2 \rho_r(\hbar\omega - E_g) \quad (5.38)$$

$$\rho_r(\hbar\omega - E_g) = \frac{1}{2\pi^2} \left( \frac{2m^*_e}{\hbar^2} \right)^{\frac{3}{2}} (\hbar\omega - E_g)^{\frac{1}{2}} \quad (5.39)$$

Therefore, the absorption coefficient depends on the momentum matrix element and the joint optical density of states. Below the band-gap energy  $E_g$ , the absorption does not occur because the photons see a forbidden band gap.

## 5.2 Interband Absorption and Gain in A Quantum Well

The central cell functions in the quantum wells are relatively unaffected by the presence of the confining potential. There are only two changes compared to bulk semiconductor, first, the nature of wavefunction for the low lying states are confined to the well region, second, the density of the state have the usual step-like form for parabolic 2-dimensional bends.

Ignore the excitonic effects due to the Coulomb interaction between electrons and holes.

Within a two-band model, the Bloch wave functions can be described by

$$\Psi_a(\mathbf{r}) = u_v(\mathbf{r}) \frac{e^{i\mathbf{k}_t \cdot \rho}}{\sqrt{A}} g_m(z) \quad (5.40)$$

for a hole wave function in the heavy-hole or a light-hole subband m. and

$$\Psi_b(\mathbf{r}) = u_c(\mathbf{r}) \frac{e^{i\mathbf{k}_t \cdot \rho}}{\sqrt{A}} \Phi_n(z) \quad (5.41)$$

for an electron in the conduction subband n. The momentum matrix element  $\mathbf{p}_{ba}$  is given by

$$\mathbf{p}_{ba} = \langle \Psi_b | \mathbf{p} | \Psi_a \rangle \approx \langle u_c | \mathbf{p} | u_v \rangle \delta_{k_t, k'_t} I_{hm}^{\text{en}} \quad (5.42)$$

where

$$I_{\text{hm}}^{\text{en}} = \int_{-\infty}^{+\infty} dz \Phi_n^*(z) g_m(z) \quad (5.43)$$

- This is the overlap integral of the conduction and valence band envelope functions
- **K**-Selection rule applied
- Take into account the quantization of the electron and hole energies  $E_a$  and  $E_b$

$$E_a = E_{\text{hm}} - \frac{\hbar^2 \mathbf{k}_t^2}{2m_h^*} \quad (5.44)$$

$$E_b = E_g + E_{\text{en}} + \frac{\hbar^2 \mathbf{k}_t^2}{2m_e^*} \quad (5.45)$$

And  $E_{\text{hm}} < 0$ ,

$$E_b - E_a = E_{\text{hm}}^{\text{en}} + E_t, E_t = \frac{\hbar^2 \mathbf{k}_t^2}{2m_e^*} \quad (5.46)$$

where

$$E_{\text{hm}}^{\text{en}} = E_g + E_{\text{en}} - E_{\text{hm}} \quad (5.47)$$

is the band edge transition energy ( $\mathbf{k}_t = 0$ ). The summations over the quantum numbers  $\mathbf{k}_a$  and  $\mathbf{k}_b$  become summations over  $(\mathbf{k}'_t, m)$  and  $(\mathbf{k}_t, n)$ . Noting in the matrix element  $\mathbf{k}_t = \mathbf{k}'_t$

$$\alpha(\hbar\omega) = C_0 \sum_{n,m} |I_{\text{hm}}^{\text{en}}|^2 \frac{2}{V} \sum_{\mathbf{k}_t} |\hat{\mathbf{e}} \cdot \mathbf{p}_{\text{cv}}|^2 \delta(E_{\text{hm}}^{\text{en}} + E_t - \hbar\omega)(f_v^m - f_c^n) \quad (5.48)$$

Use the two-dimensional joint density of states

$$\frac{2}{V} \sum_{\mathbf{k}_t} = \frac{2A}{V} \int \frac{d^2 \mathbf{k}_t}{(2\pi)^2} = \frac{1}{\pi L_z} \int_0^\infty \mathbf{k}_t d\mathbf{k}_t = \int_0^\infty d\frac{\hbar^2 \mathbf{k}_t^2}{2m_r^*} \cdot \frac{m_r^*}{\pi \hbar^2 L_z} = \int_0^\infty dE_t \rho_r^{2D} \quad (5.49)$$

$$\rho_r^{2D} = \frac{m_r^*}{\pi \hbar^2 L_z} \quad (5.50)$$

where  $A$  is the area of the cross section,  $AL_z = V$ ,  $L_z$  is an effective period of the quantum wells, and  $V$  is a volume of a period. The delta function gives the contribution at  $E_{\text{hm}}^{\text{en}} + E_t = \hbar\omega$ , and the absorption edges occur at  $\hbar\omega = E_{\text{hm}}^{\text{en}}$ . For an unpumped semiconductor,  $f_v^m = 1$  and  $f_c^n = 0$ , we have the absorption spectrum at thermal equilibrium  $\alpha_0(\hbar\omega)$

$$\alpha_0(\hbar\omega) = C_0 \sum_{n,m} |I_{\text{hm}}^{\text{en}}|^2 |\hat{e} \cdot \mathbf{p}_{\text{cv}}|^2 \rho_r^{2D} H(\hbar\omega - E_{\text{hm}}^{\text{en}}) \quad (5.51)$$

Because the integration of the delta function gives the step function, shown as  $H$  or the Heaviside step function,  $H(x) = 1$  for  $x > 0$ , and 0 for  $x < 0$ . For a symmetric quantum well, we find  $I_{\text{hm}}^{\text{en}} = \delta_{nm}$  using an infinite well model, and the absorption spectrum is

$$\begin{aligned} \alpha_0(\hbar\omega) &= C_0 |\hat{e} \cdot \mathbf{p}_{\text{cv}}|^2 \frac{m_r^*}{\pi \hbar^2 L_z} \\ C_0 &= \frac{\pi e^2}{n_r \varepsilon_0 c m_r^2 \omega} \end{aligned} \quad (5.52)$$

### 5.3 Interband Absorption and Gain in A Quantum Wire

For quantum wire structure, the confining potential also only changes the nature of wavefunction and the density of the state as in the 2-dimensional case. Also ignore the excitonic effects due to the Coulomb interaction between electrons and holes, then follow the similar procedure in 2-dimensional.

We consider a quantum wire with cross section  $a \times b$ , and the length of wire is  $L_z \gg a, b$ .

Within a semiconductor model, the valence band Bloch wave functions can be described by

$$\Psi_v(\mathbf{r}) = u_v(\mathbf{r}) \frac{e^{i\mathbf{k}_t \cdot \rho}}{\sqrt{L_z}} g_m(x, y) \quad (5.53)$$

$$g_m(x, y) = \frac{2}{\sqrt{ab}} \sin\left(\frac{m}{a}x\right) \sin\left(\frac{n}{b}y\right) \quad (5.54)$$

and the conduction band Block wave function as,

$$\Psi_c(\mathbf{r}) = u_c(\mathbf{r}) \frac{e^{i\mathbf{k}_t \cdot \rho}}{\sqrt{L_z}} \Phi_n(x, y) \quad (5.55)$$

$$\Phi_n(x, y) = \frac{2}{\sqrt{ab}} \sin\left(\frac{m' \pi}{a}x\right) \sin\left(\frac{n' \pi}{b}y\right) \quad (5.56)$$

where

$$E_v^{m' n'} = E_{v0} - \frac{\hbar^2}{2m_h^*} \left[ \left( \frac{m' \pi}{a} \right)^2 + \left( \frac{n' \pi}{b} \right)^2 + \mathbf{k}_t^2 \right] \quad (5.57)$$

$$E_c^{mn}(k_t) = E_{c0} + \frac{\hbar^2}{2m_e^*} \left[ \left( \frac{m}{a} \right)^2 + \left( \frac{n}{b} \right)^2 + \mathbf{k}_t^2 \right] \quad (5.58)$$

The momentum matrix element  $\mathbf{p}_{ba}$  is given by

$$\mathbf{p}_{ba} = \langle \Psi_b | \mathbf{p} | \Psi_a \rangle \approx \langle u_c | \mathbf{p} | u_v \rangle \delta_{k_t, k'_t} I_{hm}^{\text{en}} \quad (5.59)$$

where

$$I_{hm}^{\text{en}} = \int_{-\infty}^{+\infty} dx dy \Phi_n^*(x, y) g_m(x, y) \quad (5.60)$$

- This is the overlap integral of the conduction and valence band envelope functions
- **K**-Selection rule applied

Use the one-dimensional joint density of states,

$$\frac{2}{V} \sum_{\mathbf{k}_t} = \frac{2L_z}{V} \int \frac{d\mathbf{k}_t}{2\pi} = \frac{1}{\pi L_x L_y} \int_0^\infty \frac{1}{\mathbf{k}_t} d\mathbf{k}_t = \int_0^\infty dE_t \rho_r^{1D} \quad (5.61)$$

$$\rho_r^{1D} = \sum_{m,n} \frac{(2m_r^*)^{\frac{1}{2}}}{\pi\hbar} \frac{1}{\sqrt{(\hbar\omega - E_c^{\text{mn}})}} \quad \text{for } E > E_c^{\text{mn}} \quad (5.62)$$

$$\rho_r^{1D} = \frac{(m_r^*)^{\frac{3}{2}}}{\pi\hbar m_e^* L_x L_y} \frac{1}{\sqrt{(\hbar\omega - E_g)}} \quad (5.63)$$

The electron density is given by the occupation of the wire states, and at zero temperature it can be integrated analytically,

$$n = \sum_{m,n} \frac{(2m_r^*)^{\frac{1}{2}}}{\pi\hbar} L_x L_y \sqrt{(F_c - E_c^{\text{mn}})} \quad (5.64)$$

where  $L_z L_x L_y = V$ ,  $L_x, L_y, L_z$  are effective period of the quantum wire along different directions,  $L_z$  along the axial of the quantum wire, and  $V$  is a volume of a period. The delta function gives the contribution at  $E_{\text{hm}}^{\text{en}} + E_t = \hbar\omega$ , and the absorption edges occur at  $\hbar\omega = E_{\text{hm}}^{\text{en}}$ . For an unpumped semiconductor,  $f_v^m = 1$  and  $f_c^n = 0$ , we have the absorption spectrum at thermal equilibrium  $\alpha_0(\hbar\omega)$

$$\alpha_0(\hbar\omega) = C_0 \sum_{n,m} |I_{\text{hm}}^{\text{en}}|^2 |\hat{e} \cdot \mathbf{p}_{\text{cv}}|^2 \rho_r^{1D} H(\hbar\omega - E_{\text{hm}}^{\text{en}}) \quad (5.65)$$

Because the integration of the delta function gives the step function, shown as  $H$  or the Heaviside step function,  $H(x) = 1$  for  $x > 0$ , and 0 for  $x < 0$ . For a symmetric quantum wire, we find  $I_{\text{hm}}^{\text{en}} = \delta_{nm}$  using an infinite wire model, and the absorption spectrum is

$$\begin{aligned}
\alpha_0(\hbar\omega) &= C_0 |\hat{e} \cdot \mathbf{p}_{cv}|^2 \frac{(2m_r^*)^{\frac{1}{2}}}{\pi\omega} L_x L_y \frac{1}{\sqrt{(\hbar\omega - E_{cv}^{mn})}} \\
E_{cv}^{mn} &= E_g + \frac{\hbar^2}{2m_r^*} \left[ \left( \frac{m}{a} \right)^2 + \left( \frac{n}{b} \right)^2 \right] \\
C_0 &= \frac{\pi e^2}{n_r \varepsilon_0 c m_0^2 \omega}
\end{aligned} \tag{5.66}$$

## 5.4 Contributing Factors

The derived absorption and spontaneous emission rate are both strong function of dimensionality. Carrier confinement in core-shells, and the effect of local forces shown by band bending affects transition rates due to the following factors:

### 5.4.1 Overlap Integral

Between initial and final wave function, the confined structure altered the envelope functions and furthermore changed the overlap integral as in equation. This overlap of the conduction and valence band will have an effect on the electron transitions under electric field or external perturbation.

Where and are electron envelope function in the conduction subband n and hole envelope function in the heavy-hole or light-hole subband m correspondingly.

### 5.4.2 Oscillator Strength

The optical matrix element for the electron-to-heavy hole transition induced oscillator strength per unit length can be expressed as;

where is the three-dimensional exciton envelope function. And is the exciton wave function, where and are the ground state wave functions for electrons and heavy holes in the absence of their interaction.

Generally, different dimensionality only alters the envelope function, so if this function is included in the calculation of the oscillator strength, we should expect the oscillator strength is dependent

of the dimensionality. To be more specific, the decreasing of dimensionality will raise the oscillator strength. Esaki in paper has mentioned that the exciton oscillator strength per unit volume in the GaAs quantum well nanowire structure is about an order of magnitude larger than in bulk GaAs.

### 5.4.3 Joint Optical Density of States

As shown in the above derivation, joint optical density of state is a strong function of dimensionality which comes from the summation over wave numbers  $k$ , as shown in the equation. And as derived in former chapters, the three-dimensional joint optical density of states expresses as and the two-dimensional case and the one-dimensional shown as:

The extremely reduced effective hole mass which mentioned in Coldren's paper, from 0.118 reduced to 0.01 as in quantum wire structure, may cause by the hole band separation due to the local force or string inside the semiconductor.

## 5.5 Spacial Overlapping of confined light and electronic wavefunctions

Figure 5.1 (C) shows the FDTD-simulated electric field density of a hexagonal nanowire at y cross section (top) and x cross section (bottom). The photon energy of this mode shown as the insets of Fig. 5.1 (C) is concentrated primarily along the 6 corners and secondarily along the facets with little light in the 3D core of GaAs. Hence, we suggest that the fortuitous spatial overlap of the resonant optical modes on reduced dimensional electronic wavefunctions plays a significant role in the remarkable optoelectronic properties of core-shell nanowires. Restated, the superposition of the photon modes on reduced electronic states that form on the facets and vortices of the hexagonal CSNWs strongly enhances both upward and downward transition rates. Thus, the reduced dimensionality transition rate distinguishes the core-shell nanostructure from the optically equivalent core-only structure due to its significantly modified rate management. These nanostructures are not only excellent optical cavities, but despite their large size also provide the right reduced dimensional electronic structures which enhance optoelectronic interactions. It should be noted the present analysis is for direct optical transitions; although it can be extended to incorporate k-vector

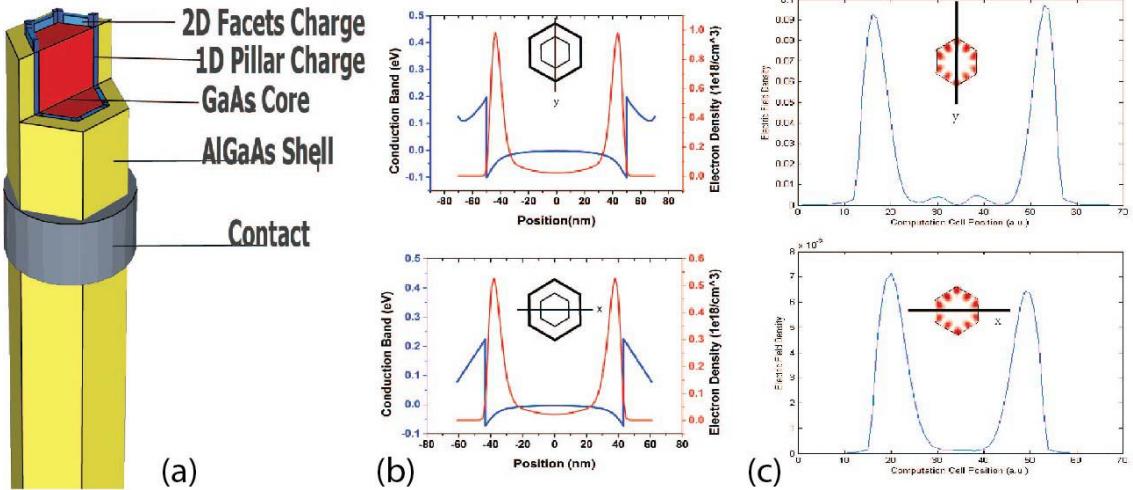


Figure 5.1 Photon Charge Distribution

changes as in phonon scattering, other important factors such as many-body interactions need to be included in a more detailed analysis.

## 5.6 Many body effects

As the reduced effective mass plays an important role in joint optical density of states and obtained from electron and hole effective mass is much larger than electron effective mass, the reduced effective mass will have a strong correlation with the hole effective mass as it decreased with the dimensionality decreasing. Thus, the reduced effective mass as it decreased with the dimensionality decreasing. Thus, the reduced effective mass will alter the joint optical density of state in the case of dimensionality changing.

The preceding theory of gain involving Fermi's Golden Rule considers each electron in isolation as it interacts with the electromagnetic field. In other words, we have used a single-particle theory to obtain the gain spectrum. In reality, there is a large density of both electrons and holes present in the system. The mutual interactions between these particles are generally referred to as many-body effects. These effects included lineshape broadening, which is related to collisions between particles and/or phonons in the crystal. In addition to this important effect, there are two other

significant consequences of many-body effects: exciton states and bandgap shrinkage. Exciton states exist primarily at low carrier densities and low temperatures, where bandgap shrinkage becomes noticeable at high carrier densities.

Under conditions of low carrier density and low temperature, it is possible for an electron and hole to orbit each other for an extended period of time, forming what is referred to as an exciton pair. Such exciton pairs have a binding energy associated with them that is equal to the energy required to separate the electron and hole. As a result, electrons that are elevated from the valence band to one of these exciton states will absorb radiation at energies equal to the bandgap less the binding energy (the bandgap will appear to be red-shifted). More significantly however, the overlap integral (and hence the matrix element) of these two-particle states can be quite large. As a result, band-to-exciton transitions tend to dominate the absorption spectrum. However, exciton states are limited to states near  $k = 0$ , and hence band-to-exciton transitions are clustered at the band edge (or subband edge). The overall effect is the appearance of very strong absorption peaks near the subband edges in quantum-well materials, and near the band edge in bulk material.

Exciton absorption peaks are clearly visible in quantum wells at room temperature for a typical GaAs QW. The first two steps in the "staircase" absorption spectrum predicted from the density of states. However, the exciton peaks riding on top of the steps, particularly the  $n = 1$  peaks, dominate the absorption spectrum. Each observed exciton peak corresponds to one of the subband transitions.

The second many-body effect occurs at high carrier densities, where the charges actually screen out the atomic attractive forces. With a weaker effective atomic potential, the single-atom electron wavefunctions of interest become less localized and the nearest-neighbor electron overlap becomes higher. The large overlap increases the width of the energy bands ( $\delta E$  is larger), reducing the gap between bands. Although this description is only qualitative, it does reveal that the bandgap should shrink with increasing carrier density.

It can also be argued theoretically that the bandgap shrinkage is inversely related to the average spacing between carriers, or (the closer the carriers are, the more their own Coulomb potentials

screen out the atomic potential). In bulk material, the average volume occupied by one carrier is inversely related to the carrier density.

The net effect of bandgap shrinkage is that as carrier density increases, the entire gain spectrum redshifts by a noticeable amount. In principle, the shift is accompanied by a slight distortion. (i.e, reshaping and enhancement) of the spectrum.

With decreasing dimensionality of the active region of an injection laser, the density of states and gain spectra become narrower, which leads to a decrease in the number of states to be filled to make the active region transparent (zero population inversion and zero gain) and to achieve lasing (gain equal to loss). Consequently, the transparency current (or inversion current) at which the gain is equal to the loss and lasing begins decrease and their temperature dependences become weaker<sup>151</sup>.

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## CHAPTER 6

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### MODELING LASING THRESHOLD

#### 6.1 History of Semiconductor Lasers

As we know, semiconductor lasers are important optoelectric devices for optical communication systems. They are essential components for building optical communication systems. There are intensive research results and achievements from beginning. In 1917, Einstein predicted the existence of spontaneous and stimulated emission by which an atom can emit radiation. The first semiconductor lasers were fabricated in 1962 using homojunctions. These lasers had high threshold current density ( $19000 A/cm^2$ ) and operated at cryogenic temperatures. The concept of heterojunction semiconductor lasers was realized in 1969 1970 with a low threshold current density ( $1600 A/cm^2$ ) operating at room temperature. These double-heterostructure diode lasers provide both carrier and optical confinements, which improve the efficiency for stimulated emission. The concept of quantum well structures for semiconductor lasers was proposed and realized experimentally in the late 1970s. The threshold current density was reduced to about  $500 A/cm^2$ , which improved the laser performance significantly.

#### 6.2 Principle of Semiconductor Lasers

The semiconductor laser (or laser diode) in its simplest form is a p-n junction of a single crystal of semiconductor material arranged in a cavity. The type and configuration of the material used determine the optical characteristics of the laser diode emission. Like others in various oscillators or wave sources, the fundamental elements in the semiconductor lasers are the following three elements:

semiconductor band structure (population inversion to provide gain mechanism), current injection and P-N junction ( external pumping to make gain sustainable) and reflector of cavity (feedback to provide coherence). The most common semiconductor lasers are including Fabry-Perot(FP) or distributed feedback (DFB)/distributed Bragg reflector (DBR).

### 6.2.1 Absorption of Light

The light and matter interaction includes absorption, spontaneous emission and stimulated emission. We first discuss the absorption of light by introducing the absorption coefficient. This is the absorption rate without considering the occupation factors. As derived in Chapter A, the absorption coefficient for 3D can be expressed as:

$$\begin{aligned}\alpha_{3D}(\hbar\omega) &= C_0 |\hat{e} \cdot \mathbf{p}_{cv}|^2 (f_v - f_c) \\ &\frac{1}{2\pi^2} \left( \frac{2m_r^*}{\hbar^2} \right)^{3/2} (\hbar\omega - E_g)^{1/2}, \\ C_0 &= \frac{\pi e^2}{n_r \epsilon_0 c m_0^2 \omega},\end{aligned}\quad (6.1)$$

and for 2D and 1D can be expressed as:

$$\begin{aligned}\alpha_{2D}(\hbar\omega) &= C_0 |\hat{e} \cdot \mathbf{p}_{cv}|^2 \frac{m_r^*}{\pi \hbar^2 L_z}, \\ \alpha_{1D}(\hbar\omega) &= C_0 |\hat{e} \cdot \mathbf{p}_{cv}|^2 \frac{(m_r^*)^{3/2}}{\pi \hbar m_e^* L_x L_y} \frac{1}{\sqrt{(\hbar\omega - E_g)}},\end{aligned}\quad (6.2)$$

The split plots of absorption coefficient for 3D, 2D and 1D are shown in Fig. 6.1. Note the unique shapes of density of states.

Then the overlay plot with multiple y axis as in Fig. 6.2 and the different scales indicating the absorption rates for 1D is 35 times larger than 3D.

### 6.2.2 Optical Gain

Following the derivation of absorption coefficient but with substitution to spontaneous emission, we can derive the gain spectrum for 3D, 2D and 1D with consideration of occupation factor by

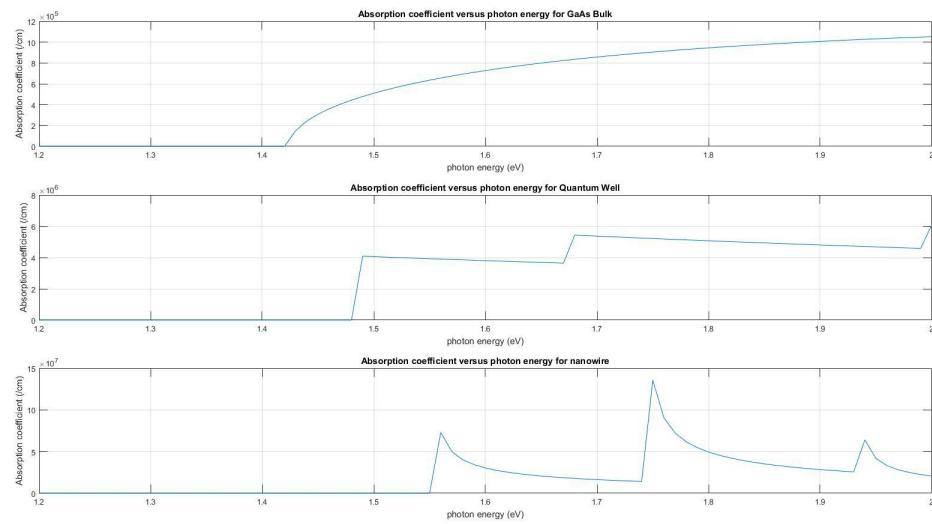


Figure 6.1 Absorption Coefficient versus Photon Energy for 1D 2D and 3D with split plot

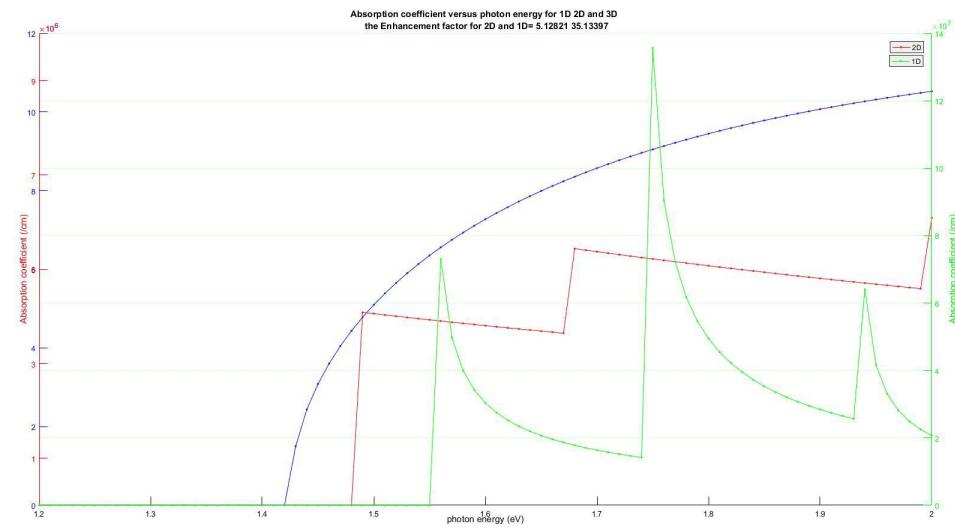


Figure 6.2 Absorption Coefficient versus Photon Energy for 1D 2D and 3D

Table 6.1. Parameters for rate euqation analysis.

Parameters	Values and Units
$A$	$1.43 \times 10^8 \text{ s}^{-1}$
$\tau_{sp}$	4 ns
$C$	$3.5 \times 10^{-30} \text{ cm}^6 - \text{s}$
$n_g$	4.2
$\Gamma$	1

Note. — This table is available in its entirety in a machine-readable form in the journal publication ?. A portion is shown here for guidance regarding its form and content.

calculating the Fermi levels.

With decreasing dimensionality of the active region of an injection laser, the density of states and gain spectra become narrower, which leads to a decrease in the number of states to be filled to make the active region transparent (zero population inversion and zero gain) and to achieve lasing (gain equal to loss). Consequently, the transparency current (or inversion current, i.e., the injection current at which the population inversion is zero) and the threshold current (injection current at which the gain is equal to the loss and lasing begins) decrease and their temperature dependences become weaker. The decrease in the threshold current and increase in its temperature stability reflect one of the main areas of development and improvement of injection lasers. Owing to the continuous nature of the carrier spectrum within the allowed subbands, the use of QWs or QWRs as active medium for optical transitions can only quantitatively improve the parameters of devices based on them compared with devices with a bulk active region.

Among the advantages of QWR lasers over the presently used QW lasers are their narrower gain spectra, much lower threshold currents, and ultrahigh temperature stability, as well as the wider possibilities for controlling their lasing wavelength.

All the parameters for rate equations analysis in table 6.1.

$$\begin{aligned}
g_{3D}(\xi) &= \frac{\sqrt{2}e^2m_r^{*3/2}p_{cv}^2}{3\pi n_r\epsilon_0 m_0^2 C\hbar^2\xi} \sqrt{(\xi - \xi_g)}(f_n(\xi_2) - f_p(\xi_1)), \\
g_{2D}(\xi) &= \frac{e^2m_r^{*3/2}p_{cv}^2}{3n_r\epsilon_0 m_0^2 C\hbar L_z\xi} (f_n(\xi_2) - f_p(\xi_1)), \\
g_{1D}(\xi) &= \frac{e^2m_r^{*3/2}p_{cv}^2}{3n_r\epsilon_0 m_0^2 C\xi L_x L_y} \frac{1}{\sqrt{(\xi - \xi_g)}} (f_n(\xi_2) - f_p(\xi_1)),
\end{aligned} \tag{6.3}$$

Now the gain spectrum respect to photon energy for 3D, 2D and 1D can be calculated in Figure 6.3.

As expected, the gain spectrum also follows the unique shapes of density of states. The Fig. 6.3(d) is the maximum gain versus electron carrier concentration varing from  $3 \times 10^{18}(cm^{-3})$  to  $3 \times 10^{19}(cm^{-3})$ .

Using parameters  $N_{tr} = 2 \times 10^{18}cm^{-3}$ ,  $N_s = 4 \times 10^{18}cm^{-3}$ , and  $g_0 = 6.11 \times 10^5 cm^{-1}$ , we fit the curve in Fig. 6.3 to build a logarithmic gain model of the form for 3D case:

$$g(N) = g_0 \ln \left( \frac{N + N_s}{N_{tr} + N_s} \right) \tag{6.4}$$

where  $N_s$  is a shift to force the natural logarithm to be finite at  $N = 0$  such that the gain equals the unpumped absorption due to the band-to-band transitions,  $N_{tr}$  is the transparency carrier density, and  $g_0$  is the gain coefficient.  $N_{tr}$  and  $g_0$  will be different for different dimensionality.

After fitting the curve in Fig. 6.4, we can calculate the threshold carrier density is  $N_{th} = 4.533 \times 10^{18}cm^{-3}$ . Then plotting the spontaneous emission rate with respect to the threshold carrier density  $N_{th}$  for 3D, 2D and 1D as following:

$$\begin{aligned}
r_{3D}^{\text{spon}}(\xi) &= \frac{n_r e^2 \xi p_{cv}^2}{\pi \epsilon_0 m_0^2 C^3 \hbar^2} \frac{m_r^{*3/2}}{2\pi^2 \hbar^3} \sqrt{(\xi - \xi_g)} f_n(\xi_2)(1 - f_p(\xi_1)), \\
r_{2D}^{\text{spon}}(\xi) &= \frac{n_r e^2 \xi p_{cv}^2}{\pi \epsilon_0 m_0^2 C^3 \hbar^2} \frac{m_r^*}{\pi \hbar^2 L_z} f_n(\xi_2)(1 - f_p(\xi_1)), \\
r_{1D}^{\text{spon}}(\xi) &= \frac{n_r e^2 \xi p_{cv}^2}{\pi \epsilon_0 m_0^2 C^3 \hbar^2} \frac{m_r^{*3/2}}{\pi \hbar m_e^* L_x L_y} \frac{1}{\sqrt{(\xi - \xi_g)}} f_n(\xi_2)(1 - f_p(\xi_1)),
\end{aligned} \tag{6.5}$$

Integrating over all the photon energy spectrum, we have the total spontaneous emission rates,  $R_{sp} =$

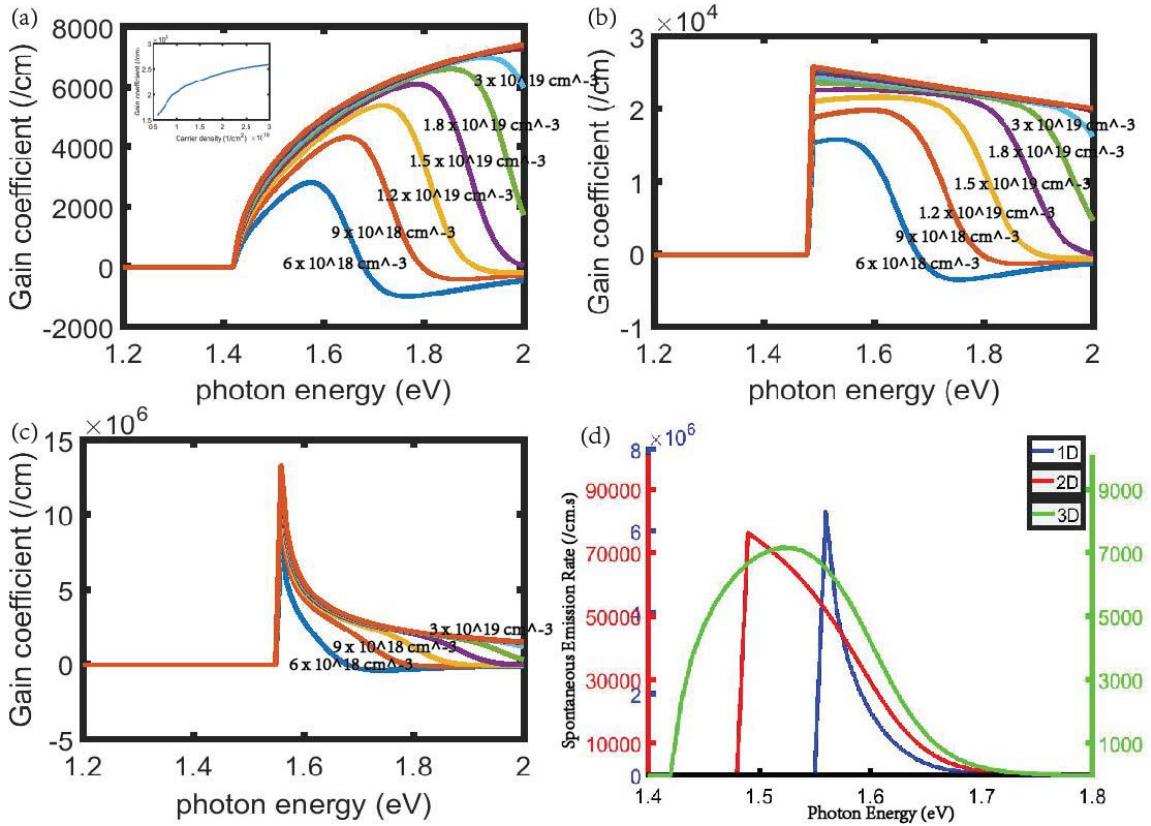


Figure 6.3 Gain Coefficient versus Photon Energy for 1D 2D and 3D

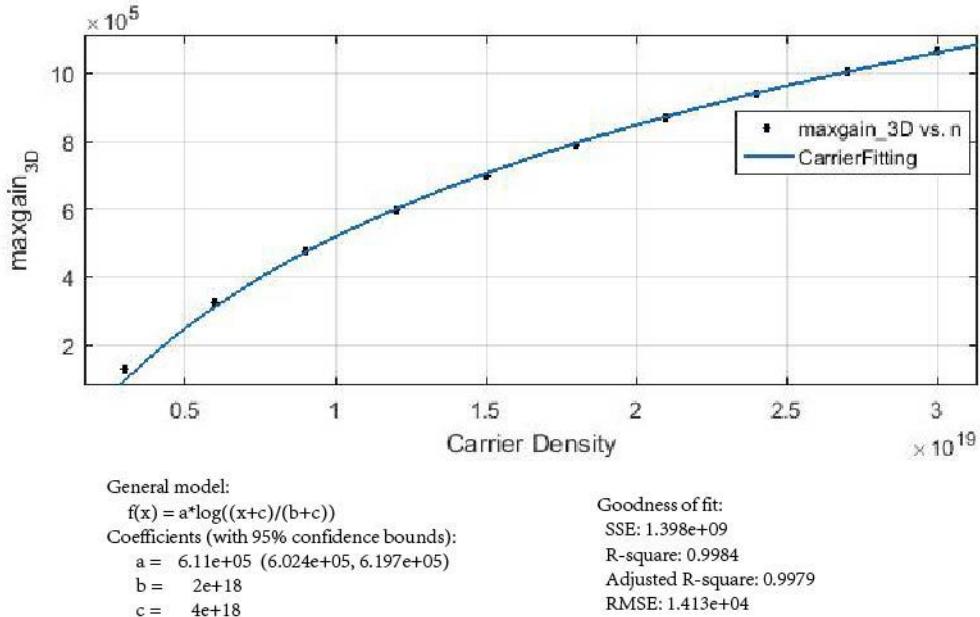


Figure 6.4 Gain Model Fitting

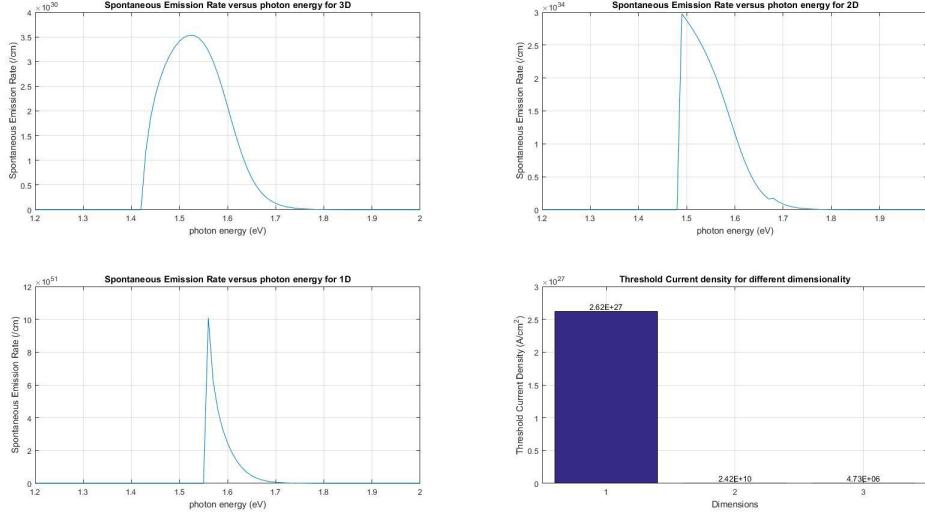


Figure 6.5 Spontaneous Emission Rate versus Photon Energy for 1D 2D and 3D

$\int_{\xi} r_{sp} d\xi$ , for different cases. Thus, the optical output power can be calculated as:  $J_{th} = qdR_{sp}|_{N_{th}}$  and plotted in the fourth part of Fig. 6.5. The total generated optical output power is 6.5 times and 175.3 times more for 2D and 1D compared to 3D case, respectively. In other words, with the same amount of carriers injected either by optical pumping or electrical injection, highly confined electronic structure can easily produce more than two orders of magnitude more light compared to less confined structure.

### 6.3 Modeling of Semiconductor Lasers

From the general formulations through the rate equations and wave equations based on the As we know, from different aspects of the same physics of the energy conservation, there are two basic classical methods to model the operation of semiconductor lasers. The first method applies the concept of photo/electron particle exchange with the abstract optical parameters and is suitable for the FP lasers. For the DBR/DFB lasers, due to strong non-uniformities of index distribution. The interaction between electromagnetic fields and electric particles has been considered, which . Indeed, those two methods are wholly compatible with one another. In this section, because the

nanowire based lasers have net propagating resonance mode in the axial direction and the resonance modes are very similar to the FP modes, we employ the first method: the standard rate equation approach.

Three fundamental elements in the semiconductor lasers: semiconductor band structure, current injection, and cavity. The former two are related to the material and junction structure, and the latter is related to the laser structure. For semiconductor lasers, the key in the modeling is to deal with the interaction between electromagnetic fields and gain medium. The basic procedure of modeling of semiconductor lasers: Due to the complexity of the rate equation and coupling between carrier and photon density, the coupling rate equations are further solved by numerical methods such as the standing-wave approach (in frequency domain) and the traveling-wave approach (in time domain). The standing-wave approach is based on the assumption that the temporal and the spatial dependence of field distributions of the cavity modes are separable. As such, the dynamics is considered in the modal amplitudes. Consequently, the standing-wave approach is valid only when the photon lifetime is much shorter than the characteristic time of the laser dynamics. The traveling-wave approach, on the other hand, makes no assumptions about the cavity modes. Rather, it solves the time-dependent coupled-wave equations for the forward and the backward traveling waves directly and therefore is valid even the laser cavity has relatively small Q-factor and/or the characteristic time of the laser dynamics is very short. Another advantage of the traveling-wave model is that it can be readily applied to laser diodes operated with multiple cavity modes, for which the standing-wave model may have difficulty in finding the complex roots corresponding to each mode.

## 6.4 Laser Rate Equations

We start with the governing equations of carrier density and photon density in the active region which is governed by a dynamic process.

$$\begin{aligned}\frac{dN}{dt} &= \frac{\eta_i I}{qV} - \frac{N}{\tau} - R_{st}, \\ \frac{dN_p}{dt} &= \Gamma v_g g N_p + \Gamma \beta_{sp} R_{sp} - \frac{N_p}{\tau_p},\end{aligned}\tag{6.6}$$

where  $\beta_{sp}$  is the spontaneous emission factor, defined as the percentage of the total spontaneous emission coupled into the lasing mode. And it is just the reciprocal of the number of available optical modes in the bandwidth of the spontaneous emission for uniform coupling to all modes. The  $g$  is Incremental gain per unit length.

The first term of equation 1 is the rate of injected electrons  $G_{gen} = \Gamma_i I / qV$ ,  $\Gamma_i I / q$  is the number of electrons per second being injected into the active region, where  $V$  is the volume of the active region. The rest terms are the rate of recombining of electrons per unit volume in the active region. There are several mechanisms should be considered, including a spontaneous recombination rate,  $R_{sp}$ , a nonradiative recombination rate,  $R_{nr}$ , a carrier leakage rate,  $R_l$  and a net stimulated recombination,  $R_{st}$ , including both stimulated absorption and emission. Which looks like:

$$R_{rec} = R_{sp} + R_{nr} + R_l + R_{st}\tag{6.7}$$

The above equation used input current intensity,  $I$ , for electrically injected lasing situation, however, if optical pump used as the lasing source, then we need to rewrite the governing equations.

$$\begin{aligned}\frac{dN}{dt} &= \frac{\eta_i P}{qV} - \frac{N}{\tau} - R_{st}, \\ \frac{dN_p}{dt} &= \Gamma v_g g N_p + \Gamma \beta_{sp} R_{sp} - \frac{N_p}{\tau_p},\end{aligned}\tag{6.8}$$

$P$  is the optical pump used for exciting nano-cavity laser emission and is time-dependent of the form  $P_p \operatorname{sech}^2(\frac{1.76t}{\delta t})$ , where  $P_p$  is the peak power amplitude, and  $\delta t$  is the time pulse width.

The cavity loss can be characterized by a photon decay constant or lifetime,  $\tau_p$ , and the gain necessary to overcome losses, and thus reach threshold. By assuming steady-state conditions (i.e.  $dN_p/dt = 0$ ), and solving for this steady-state or threshold gain,  $g_{th}$ , where the generation term equals the recombination term for photons. We assume only a small fraction of the spontaneous emission is coupled into the mode (i.e.  $\beta_{sp}$  is quite small), then the second term can be neglected, and we have the solution:

$$\Gamma g_{th} = \frac{1}{v_g \tau_p} = <\alpha_i> + \alpha_m \quad (6.9)$$

The product,  $\Gamma g_{th}$ , is referred to as the threshold modal gain because it now represents the net gain required for the mode as a whole, and it is the mode as a whole that experiences the cavity loss.  $<\alpha_i>$  is the average internal loss, and  $\alpha_m$  is the mirror loss if we considered an in-plane wave laser.

$$R_{rec} = R_{sp} + R_{nr} + R_l + R_{st} \quad (6.10)$$

The first three terms on the right refer to the natural or unstimulated carrier decay processes. The fourth one,  $R_{st}$ , require the presence of photon.

Then, recognizing that  $(R_{sp} + R_{nr} + R_l) = AN + BN^2 + CN^3$  depends monotonically on  $N$ , we observe from eq 2.34 that above threshold  $(R_{sp} + R_{nr} + R_l)$  will also clamp at its threshold value, given by Eq 2.35. Thus, we can substitute Eq 2.35 into the carrier rate equation, eq 2.16 to obtain a new above threshold carrier rate equations,

$$\frac{dN}{dt} = \eta_i \frac{(I - I_{th})}{qV} - v_g g N_p, \quad (I > I_{th}) \quad (6.11)$$

We also calculate a steady-state photon density above threshold where  $g = g_{th}$ ,

$$N_p = \frac{\eta_i(I - I_{th})}{qv_g g_{th} V} \quad (\text{steady state}) \quad (6.12)$$

To obtain the power out, we first construct the stored optical energy in the cavity,  $E_{os}$ , by multiplying the photon density,  $N_p$ , by the energy per photon,  $hv$ , and the cavity volume,  $V_p$ . That is  $E_{os} = N_p h v V_p$ . Then, we multiply this by the energy loss rate through the mirrors,  $v_g \alpha_m = \frac{1}{\tau_m}$ , to get the optical power output from the mirrors,

$$P_0 = v_g \alpha_m N_p h v V_p \quad (6.13)$$

Substituting from , and using  $\Gamma = V/V_p$ ,

$$P_0 = \eta_i \left( \frac{\alpha_m}{\langle \alpha_i \rangle + \alpha_m} \right) \frac{hv}{q} (I - I_{th}), \quad (I > I_{th}) \quad (6.14)$$

We can get the threshold carrier density

$$N_{th} = N_{tr} e^{g_{th}/g_0 N} = N_{tr} e^{(\langle \alpha_i \rangle + \alpha_m)/\Gamma g_0 N} \quad (6.15)$$

Using the polynomial fit for the recombination rates, and recognizing that for the best laser material the recombination at threshold is dominated by spontaneous recombination, we have,  $I_{th} \cong BN_{th}^2 qV/\eta_i$ , Thus

$$I_{th} \cong \frac{qVBN_{tr}^2}{\eta_i} e^{(\langle \alpha_i \rangle + \alpha_m)/\Gamma g_0 N} \quad (6.16)$$

where for most  $III - V$  materials the bimolecular recombination coefficient,  $B \sim 10^{-10} \text{ cm}^3/\text{s}$ .

Reduce the transparency value and increase the differential gain of the active materials.

It is desirable to reduce the cavity loss ( $\langle \alpha_i \rangle + \alpha_m$ ) and volume,  $V$ , in order to retaining a reasonably large confinement factor,  $\Gamma$ .

## 6.5 Linewidth Enhancement Factor

Electrons and holes frequently interact with other carriers and with phonons, thereby changing their energy within the sub-band. Such intra-band scatter events happen about every 0.1 ps, much more often than band-to-band recombination events. Thus, scattering leads to an uncertainty of the electron energy, which can be accounted for by introducing a symmetrical linewidth broadening function  $L$  into the gain formula. This convolution integral means that gain at the photon energy can now receive contributions from electron transitions within subbands.

In fact, positive gain is now possible even for photon energies slightly below the bandgap. Cauchy himself exploited such a density function in 1827, with infinitesimal scale parameter, in defining a Dirac delta function, while among physicists, it is known as the Lorentzian line shape function  $L$  with the half-width. This function is based on the assumption that the occupation probability of an electron state decays proportionally to  $\exp(-t/\tau)$ . The Fourier transformation of this exponential function into the energy domain.  $\Gamma$  is the average of the broadening in the conduction and in the valence band. The full linewidth  $2\Gamma$  is related to the average intra-band scattering time, which includes scattering events in the conduction band and valence band. For each band, linewidth contributions from different scattering processes are adding up.

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## CHAPTER 7

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### CONCLUSIONS AND FUTURE RESEARCH

As mentioned previously, communication of information, together with storage and computation form a grand challenge of the information age. Recently, the analysis of big data has become the engine for societal, financial, scientific, and technological endeavors. This demands an infrastructure that is capable of fast and reliable high volume data processing. Traditionally, this requirement was fulfilled by silicon technology. However, silicon-based technology has its own limitations, such as speed limit and heat dissipation problem. In order to process high volume data, we need data computation, storage and communication work as three fundamental functions of a computation cell. And core-shell nanowires will play an important role in this regime with their extraordinary optical properties.

In conclusion, fabrication techniques, electrical and optical properties of core-shell nanowires grown on GaAs or Si substrates were discussed here emphasizing the analysis of resonant optical modes which depend both radially and axially on the geometries of the nanowires. This shows how such sub-wavelength structures can form optical cavities as-grown, without needing sophisticated facet mirrors. In addition, we show how the fortuitous overlap of the reduced dimensional electronic wave functions and the photonic modes is responsible for the extraordinary optoelectronic properties of core-shell nanowires. Such nano-structures have been developed on heterogeneous substrates, particularly silicon, and as such becoming an important component in the next generation of photonic integrated circuits which are particularly useful in meeting the grand challenge of low energy and fast speed computation.

## 7.1 Contributions of this dissertation

In this dissertation, we designed and fabricated the CSNWs based heterostructure devices, measured and simulated their opto-electronic properties, and compared it with bulk structures. The static behavior simulations, including 2-D potential profile, electric field distributions, and carrier concentration, were performed with commercially available software. The light confinement and distribution in the CSNWs was investigated by FDTD simulation. The simulation revealed the transverse and longitudinal plane waves in the resonance frequency enhanced the optical confinement of these sub-micron scale cavities.

We showed that how low dimensional electron density distribution change the optical transition rates when a small perturbation is introduced by light which results in large enhancement of optical properties.

In addition, we designed a CSNW based laser and modeled its static and dynamic lasing behavior by calculating the optical gain and threshold current density, demonstrated that how reduced dimensional electron states enhance the overall gain and emission efficiency compared to its bulk counterpart.

The major contributions of this thesis are (1) design, fabricate and characterize the hexagonal CSNWs grown on Si or GaAs substrates, revealing enhanced optical properties, such as absorption, emission and lasing; (2) simulation and analysis of light confinement and propagation mechanism in CSNWs; (3) simulation and analysis of electron distribution in the hexagonal CSNWs; (4) derived dimensional dependent band-to-band transition rates and proposed the spacial overlapping of the confined light with reduced electronic wave function greatly enhanced the optical transition rates; (5) modeled and calculated the optical gain and output power in order to justify that lower dimensional electron states will facilitate the lasing behaviors of CSNW based laser and produced more light compare to their bulk counterparts.

## 7.2 Outline of the future work

### 7.2.1 Plasmonic Effect

Low dimensional electron gases exist at the heterointerfaces of core-shell nanowires (CSNWs). For example, the GaAs/AlGaAs CSNWs typically form a hexagonal structure in which six (6) pillars of 1D charge at the vortices, and six (6) sheets of 2D charge at facets are formed<sup>119</sup>. At the same time, nanowires (NW) have also been shown to be capable of confining light in their sub-wavelength nanostructure, supporting photonic modes, and producing resonant cavities without the need for polished end facets. We have previously shown how the electronic wave functions that are thus formed affect the optical transition rates, resulting in orders of magnitude enhancement in absorption and emission of light. Here we propose the plasmonic effects of the confined charge on the optical properties of CSNWs.

The finite difference time domain (FDTD) simulations identify the surface plasmon resonance modes which affect light confinement in hexagonal CSNWs, and help form a high quality factor resonant cavity. We compare regular CSNW, with a) wires covered with metal which produces surface plasmon-polaritons (SPP); b) NWs covered with metal that is sandwiched between the core and the outer, shell; and c) two-dimensional electron gas (2DEG) which embedded at the heterointerface of CSNWs. Results show that the 2DEG behaves similarly to an embedded metallic surface, allowing for highly localized light confinement in these wires without the need for vertical structures such as Bragg mirrors commonly used in vertical cavity surface emitting lasers (VCSELs). Besides affecting the cavity, the 2DEG enhances the transition rates due to the plasmon-electron interaction, facilitating not only photonic stimulated emission and lasing, but also surface plasmon amplification by stimulated emission of radiation<sup>152</sup>.

The electromagnetic wave traveling of the Surface Plamon Polariton (SPP) involves both charge motion in electron reservoir (e.g., metal, graphene and 2DEG) and waves in the dielectric or air. Instead of using any metallic materials, Core-Shell nanowires (CSNWs) can naturally form two-dimensional electron gas (2DEG) at the heterojunction interface and even large one-dimensional

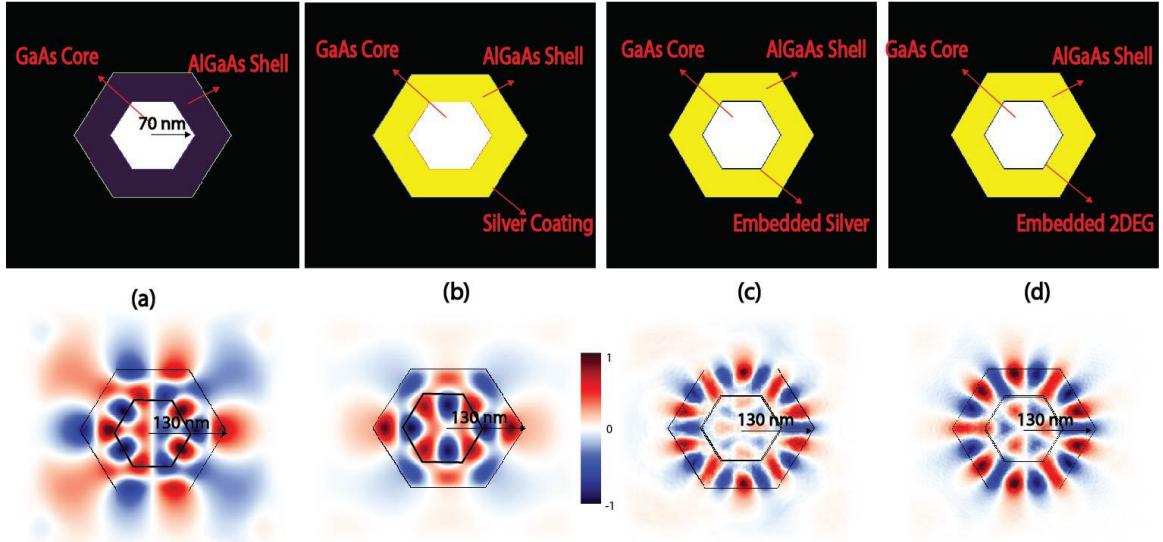


Figure 7.1 An FDTD-simulated electric field profile (linear scale) of (a) a hexagonal core-shell nanowire (CSNW), (b) photonic modes are affected by plamonic modes in a CSNW covered with silver coating, (c) CSNW with embedded silver layer between the core and the shell; (d) plamonic and photonic modes of CSNW with embedded 2DEG show similar effects compared to embedded metal. The black boundaries represent the interface between layers of the structure.

pillar of charge at the corners of their hexagonal facets.

Figure 7.1 shows the FDTD-simulated electric field profile (linear scale) in the transverse plane of (a) CSNW; (b) CSNW with silver coating; (c) CSNW with and embedded silver layer between the core and the shell; (d) CSNW with 2DEG at the hetero-interface. As shown in Fig 7.1, coating the wire with metal introduces plamonic modes in the structure that enhance light confinement. Metal embedded between the core and the shell has similar effect. Importantly, we observe that similar plamonic features can be obtained due to the 2DEG that is embedded in CSNW<sup>153</sup>.

### 7.2.2 Monolithic Integration on PIC

Recently, the increasing demand for high-speed low-power computation and communication has driven the growth of photonics integrated circuit (PIC) technology with projected market size of a billion dollars by 2018 . Silicon photonics have received significant attention as it benefits from well-established complementary metal-oxide-semiconductor (CMOS) technology. Lack of an effi-

cient silicon-based light source and photodetector, has motivated development of technologies for heterogeneous integration of efficient III-V semiconductor light sources and detector with silicon chips. Here we present core-shell nanowires (CSNWs) as versatile low-dimensional optoelectronic systems as a replacement to their conventional thin film counterparts in heterogeneous integration in silicon photonics. These CSNWs have extraordinary performance in light generation, absorption, light modulation, energy generation, and high-speed optical detection. Finally, we elaborate on a vision for a low-cost high-performance silicon photonics chip based on a core-shell nanowire platform. In this scheme, CSNWs are applied as high-speed low-power optical detectors, light source, and waveguides.

In order to process high volume data, we need data computation, storage, and communication to work in concert as the three fundamental functions of a computation cell. As schematically shown in Fig. 7.2, a monolithic nanosystem may be envisioned, which incorporates NWs as waveguides, detectors, photovoltaic cells, antennas, modulators, (photo)capacitors, LEDs and lasers. These components may be incorporated in circuit layers, such as network-on-chip. Different layers can communicate using NW through-silicon vias (TSVs). Similar low-power/high-performance advantages can be realized through achievement of high interconnect densities on the 2.5D through-Si-interposer (TSI) as reported in reference<sup>154</sup>

Performance enhancement of CSNWs can be attributed to the formation of confined quasi-one-dimensional electron gas at the vortices, and two-dimensional electron gas at the facets of the hexagonally shaped GaAs/AlGaAs core-shell hetero-interface. These reduced dimensional confined charge plasma affect optical transition rates, facilitate population inversion, and collect optically generated electrons and holes before they transit to the contacts. Additionally these plasmons, which are unique to CSNWs, affect waveguiding and optical cavity properties of CSNWs and can be used as waveguides, modulators and photocapacitors.

The proposed integrated photonic platform is schematically depicted at the bottom part of Fig. 7.2 with multiple key components implemented through utilizing core-shell nanowires. This monolithic

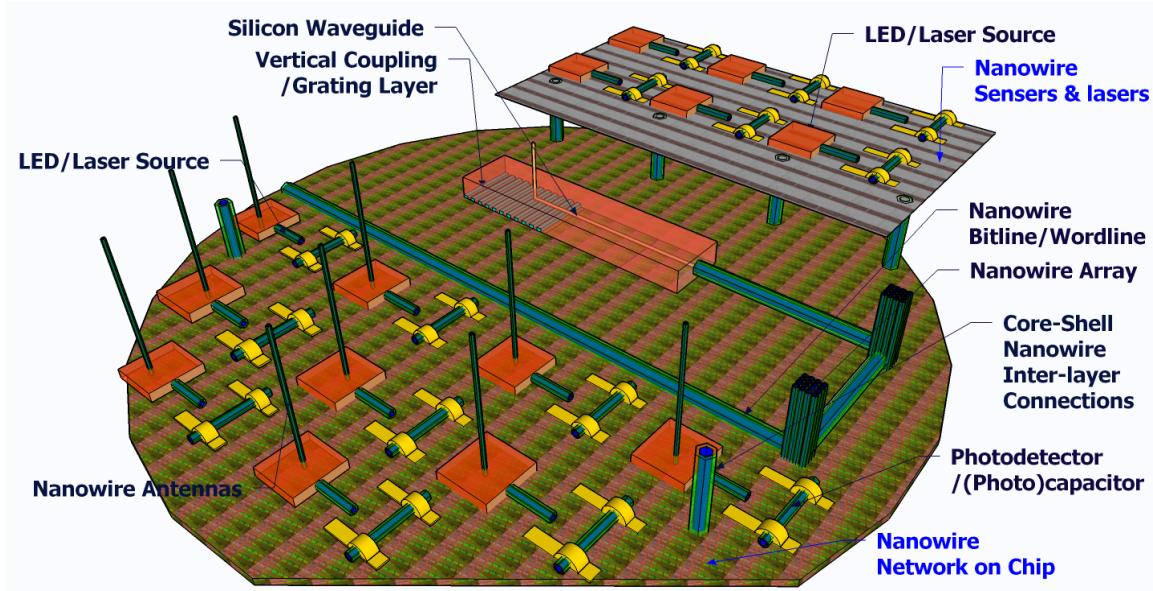


Figure 7.2 Schematic depiction of an optoelectronic nanosystem may include key components such as NW LED/laser source, photodetector/photocapacitor, NW antennas, and NW-enabled network-on-chip integrated on silicon.

nanosystem incorporates CSNWs as waveguides, detectors, photovoltaic cells, antennas, modulators, LEDs, and lasers. These components may be incorporated in circuit layers, such as networks on chip. Additionally, they can be used for 3D integration using NW through-silicon vias (TSVs). Such a circuit may compete with manufacturing methods such as flip-chip bonding and achieves further miniaturization by incorporating high-performance nanowires in vertical architectures to replace large surface area thin film structures such as vertical cavity surface emitting lasers (VCSELs).

In conclusion, CSNW demonstrate unique combination of plasmonic, photonic, and electronic properties which makes them versatile high-performance optoelectronic devices including Lasers, LEDs, photodetectors, solar cells, waveguides, and optical amplifiers. Since they can be grown from a wide range of material including GaAs, InP, and GaN, at different directions and on foreign substrates such as oxides, Graphene, Si, and III-Vs, they offer a competitive platform for photonic integrated circuits, and specifically for heterogeneous integration in silicon photonics chips, photodetectors/photocapacitors, antennas and waveguides.

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## BIBLIOGRAPHY

- [1] T. Nobis and M. Grundmann, “Low-order optical whispering-gallery modes in hexagonal nanocavities,” *Physical Review A*, vol. 72, no. 6, p. 063806, 2005.
- [2] R. Chen, T. T. D. Tran, K. W. Ng, W. S. Ko, L. C. Chuang, F. G. Sedgwick, and C. Chang-Hasnain, “Nanolasers grown on silicon,” *Nature Photonics*, vol. 5, no. 3, pp. 170–175, 2011.
- [3] S. Sun, Z. Fan, Y. Wang, and J. Haliburton, “Organic solar cell optimizations,” *Journal of materials science*, vol. 40, no. 6, pp. 1429–1443, 2005.
- [4] J. Perlin, *From space to earth: the story of solar electricity*. Earthscan, 1999.
- [5] M. Razeghi and A. Rogalski, “Semiconductor ultraviolet detectors,” *Journal of Applied Physics*, vol. 79, no. 10, pp. 7433–7473, 1996.
- [6] A. Rogalski, “Infrared detectors: an overview,” *Infrared Physics & Technology*, vol. 43, no. 3, pp. 187–210, 2002.
- [7] E. Chen and A. Murphy, *Broadband optical modulators: science, technology, and applications*. CRC press, 2011.
- [8] J. A. Schuller, E. S. Barnard, W. Cai, Y. C. Jun, J. S. White, and M. L. Brongersma, “Plasmonics for extreme light concentration and manipulation,” *Nature materials*, vol. 9, no. 3, pp. 193–204, 2010.
- [9] H. Spanggaard and F. C. Krebs, “A brief history of the development of organic and polymeric photovoltaics,” *Solar Energy Materials and Solar Cells*, vol. 83, no. 2, pp. 125–146, 2004.
- [10] E. F. Schubert and J. K. Kim, “Solid-state light sources getting smart,” *Science*, vol. 308, no. 5726, pp. 1274–1278, 2005.
- [11] E. F. Schubert, T. Gessmann, and J. K. Kim, *Light emitting diodes*. Wiley Online Library, 2005.
- [12] W. W. Chow, S. W. Koch, and M. I. Sargent, *Semiconductor-laser physics*. Springer Science & Business Media, 2012.
- [13] E. Yablonovitch, “Inhibited spontaneous emission in solid-state physics and electronics,” *Physical review letters*, vol. 58, no. 20, p. 2059, 1987.
- [14] Z. Alferov, “Double heterostructure lasers: early days and future perspectives,” *IEEE Journal of Selected Topics in Quantum Electronics*, vol. 6, no. 6, pp. 832–840, 2000.
- [15] Y. Xia, P. Yang, Y. Sun, Y. Wu, B. Mayers, B. Gates, Y. Yin, F. Kim, and H. Yan, “One-dimensional nanostructures: synthesis, characterization, and applications,” *Advanced materials*, vol. 15, no. 5, pp. 353–389, 2003.
- [16] R. Yan, D. Gargas, and P. Yang, “Nanowire photonics,” *Nature Photonics*, vol. 3, no. 10, pp. 569–576, 2009.
- [17] R. G. Hobbs, N. Petkov, and J. D. Holmes, “Semiconductor nanowire fabrication by bottom-up and top-down paradigms,” *Chemistry of Materials*, vol. 24, no. 11, pp. 1975–1991, 2012.

- [18] Y. Wu and P. Yang, "Direct observation of vapor- liquid- solid nanowire growth," *Journal of the American Chemical Society*, vol. 123, no. 13, pp. 3165–3166, 2001.
- [19] W. Lu and C. M. Lieber, "Nanoelectronics from the bottom up," *Nature materials*, vol. 6, no. 11, pp. 841–850, 2007.
- [20] M. H. Huang, S. Mao, H. Feick, H. Yan, Y. Wu, H. Kind, E. Weber, R. Russo, and P. Yang, "Room-Temperature Ultraviolet Nanowire Nanolasers," *Science*, vol. 292, no. 5523, pp. 1897–1899, 2001.
- [21] I. Park, Z. Li, A. P. Pisano, and R. S. Williams, "Top-down fabricated silicon nanowire sensors for real-time chemical detection," *Nanotechnology*, vol. 21, no. 1, p. 015501, 2009.
- [22] P. Yang, H. Yan, S. Mao, R. Russo, J. Johnson, R. Saykally, N. Morris, J. Pham, R. He, and H.-J. Choi, "Controlled growth of ZnO nanowires and their optical properties," *Advanced Functional Materials*, vol. 12, no. 5, p. 323, 2002.
- [23] A. I. Persson, M. W. Larsson, S. Stenström, B. J. Ohlsson, L. Samuelson, and L. R. Wallenberg, "Solid-phase diffusion mechanism for gaas nanowire growth," *Nature materials*, vol. 3, no. 10, pp. 677–681, 2004.
- [24] A. I. Hochbaum, R. Fan, R. He, and P. Yang, "Controlled growth of si nanowire arrays for device integration," *Nano letters*, vol. 5, no. 3, pp. 457–460, 2005.
- [25] Y. Wu and P. Yang, "Germanium nanowire growth via simple vapor transport," *Chemistry of Materials*, vol. 12, no. 3, pp. 605–607, 2000.
- [26] S. Schmitt-Rink, D. Chemla, and D. Miller, "Linear and nonlinear optical properties of semiconductor quantum wells," *Advances in Physics*, vol. 38, no. 2, pp. 89–188, 1989.
- [27] M. Yazawa, M. Koguchi, and K. Hiruma, "Heteroepitaxial ultrafine wire-like growth of inas on gaas substrates," *Applied Physics Letters*, vol. 58, no. 10, pp. 1080–1082, 1991.
- [28] L. Cao, J.-S. Park, P. Fan, B. Clemens, and M. L. Brongersma, "Resonant Germanium Nanoantenna Photodetectors," *Nano Letters*, vol. 10, no. 4, pp. 1229–1233, 2010.
- [29] L. Cao, J. S. White, J.-S. Park, J. A. Schuller, B. M. Clemens, and M. L. Brongersma, "Engineering light absorption in semiconductor nanowire devices," *Nature Materials*, vol. 8, no. 8, pp. 643–647, 2009.
- [30] M. Royo, C. Segarra, A. Bertoni, G. Goldoni, and J. Planelles, "Aharonov-Bohm oscillations and electron gas transitions in hexagonal core-shell nanowires with an axial magnetic field," *arXiv preprint arXiv:1501.06694*, 2015.
- [31] M. Currie, Z. Wang, P. Dianat, P. Prete, I. Miccoli, N. Lovergne, and B. Nabet, "Large Light Emission Enhancement in GaAs/AlGaAs CoreShell Nanowires," in *International Conference on One-Dimensional Nanomaterials, ICON2013*, (Annecy, France), 2013.
- [32] Y. W. Heo, B. S. Kang, L. C. Tien, D. P. Norton, F. Ren, J. R. La Roche, and S. J. Pearton, "UV photoresponse of single ZnO nanowires," *Appl. Phys. A*, vol. 80, no. 3, pp. 497–499, 2004.
- [33] J. H. He, C. L. Hsin, J. Liu, L. J. Chen, and Z. L. Wang, "Piezoelectric gated diode of a single zno nanowire," *Advanced Materials*, vol. 19, no. 6, pp. 781–784, 2007.
- [34] X. Duan, Y. Huang, R. Agarwal, and C. M. Lieber, "Single-nanowire electrically driven lasers," *Nature*, vol. 421, no. 6920, pp. 241–245, 2003.
- [35] K. Moratis, S. L. Tan, S. Germanis, C. Katsidis, M. Androulidaki, K. Tsagaraki, Z. Hatzopoulos, F. Donatini, J. Cibert, and Y.-M. Niquet, "Strained GaAs/InGaAs Core-Shell Nanowires for Photovoltaic Applications," *Nanoscale Res Lett*, vol. 11, no. 1, pp. 1–7, 2016.

- [36] Z. Wang, M. Currie, P. Prete, N. Lovergne, and B. Nabet, "Lasing from As Grown GaAs-AlGaAs Core-Shell Nanowires up to Room Temperature," in *Frontiers in Optics 2015*, (San Jose, California), p. LTh2I.4, Optical Society of America, 2015.
- [37] B. Badada, T. Shi, H. Jackson, L. Smith, Q. Gao, H. H. Tan, and C. Jagadish, "Photocurrent spectroscopy of single GaAs/AlGaAs core-multishell nanowire devices," in *Device Research Conference (DRC), 2015 73rd Annual*, pp. 81–82, 2015.
- [38] O. Takehiro, A. Keita, T. Kohei, W. Takao, and S. Kazuhiko, "Emission wavelength control of self-catalytic InP/GaInAs/InP core–multishell nanowire on InP substrate grown by metal organic vapor phase epitaxy," *Japanese Journal of Applied Physics*, vol. 55, no. 3, p. 031201, 2016.
- [39] Y. Li, J. Xiang, F. Qian, S. Gradecak, Y. Wu, H. Yan, D. A. Blom, and C. M. Lieber, "Dopant-free gan/alm/algan radial nanowire heterostructures as high electron mobility transistors," *Nano letters*, vol. 6, no. 7, pp. 1468–1473, 2006.
- [40] H. Sakaki, "Scattering suppression and high-mobility effect of size-quantized electrons in ultrafine semiconductor wire structures," *Japanese Journal of Applied Physics*, vol. 19, no. 12, p. L735, 1980.
- [41] J. Xiang, W. Lu, Y. Hu, Y. Wu, H. Yan, and C. M. Lieber, "Ge/si nanowire heterostructures as high-performance field-effect transistors," *Nature*, vol. 441, no. 7092, pp. 489–493, 2006.
- [42] N. Singh, A. Agarwal, L. Bera, T. Liow, R. Yang, S. Rustagi, C. Tung, R. Kumar, G. Lo, N. Balasubramanian, *et al.*, "High-performance fully depleted silicon nanowire (diameter/spl les/5 nm) gate-all-around cmos devices," *IEEE Electron Device Letters*, vol. 27, no. 5, pp. 383–386, 2006.
- [43] S. D. Suk, S.-Y. Lee, S.-M. Kim, E.-J. Yoon, M.-S. Kim, M. Li, C. W. Oh, K. H. Yeo, S. H. Kim, D.-S. Shin, *et al.*, "High performance 5nm radius twin silicon nanowire mosfet (tsnwfet): fabrication on bulk si wafer, characteristics, and reliability," in *Electron Devices Meeting, 2005. IEDM Technical Digest. IEEE International*, pp. 717–720, IEEE, 2005.
- [44] Z. Liu, Y. Zhan, G. Shi, S. Moldovan, M. Gharbi, L. Song, L. Ma, W. Gao, J. Huang, R. Vajtai, F. Banhart, P. Sharma, J. Lou, and P. M. Ajayan, "Anomalous high capacitance in a coaxial single nanowire capacitor," *Nat Commun*, vol. 3, p. 879, 2012.
- [45] J. Wallentin, J. M. Persson, J. B. Wagner, L. Samuelson, K. Deppert, and M. T. Borgstrom, "High-performance single nanowire tunnel diodes," *Nano Lett*, vol. 10, no. 3, pp. 974–979, 2010.
- [46] Y. Heo, L. Tien, D. Norton, S. Pearton, B. Kang, F. Ren, and J. LaRoche, "Pt/ zno nanowire schottky diodes," *Applied physics letters*, vol. 85, no. 15, pp. 3107–3109, 2004.
- [47] K. H. Li, X. Liu, Q. Wang, S. Zhao, and Z. Mi, "Ultralow-threshold electrically injected AlGaN nanowire ultraviolet lasers on Si operating at low temperature," *Nat Nano*, vol. 10, no. 2, pp. 140–144, 2015.
- [48] W. Wei, Y. G. Liu, X. Zhang, Z. Wang, and X. M. Ren, "Evanescent-wave pumped room-temperature single-mode GaAs/AlGaAs core-shell nanowire lasers," *Applied Physics Letters*, vol. 104, no. 22, p. 223103, 2014.
- [49] D. Saxena, S. Mokkapati, P. Parkinson, N. Jiang, Q. Gao, H. H. Tan, and C. Jagadish, "Optically pumped room-temperature GaAs nanowire lasers," *Nature Photonics*, vol. 7, no. 12, pp. 963–968, 2013.
- [50] B. Mayer, D. Rudolph, J. Schnell, S. Morkotter, J. Winnerl, J. Treu, K. Muller, G. Bracher, G. Abstreiter, G. Koblmuller, and J. J. Finley, "Lasing from individual GaAs-AlGaAs core-shell nanowires up to room temperature," *Nat Commun*, vol. 4, p. 2931, 2013.

- [51] B. Hua, J. Motohisa, Y. Kobayashi, S. Hara, and T. Fukui, "Single GaAs/GaAsP coaxial core-shell nanowire lasers," *Nano Letters*, vol. 9, no. 1, pp. 112–116, 2009.
- [52] R. Agarwal, C. J. Barrelet, and C. M. Lieber, "Lasing in Single Cadmium Sulfide Nanowire Optical Cavities," *Nano Letters*, vol. 5, no. 5, pp. 917–920, 2005.
- [53] S. Gradečak, F. Qian, Y. Li, H.-G. Park, and C. M. Lieber, "GaN nanowire lasers with low lasing thresholds," *Applied Physics Letters*, vol. 87, no. 17, p. 173111, 2005.
- [54] S. Zhao, A. T. Connie, M. H. Dastjerdi, X. H. Kong, Q. Wang, M. Djavid, S. Sadaf, X. D. Liu, I. Shih, H. Guo, and Z. Mi, "Aluminum nitride nanowire light emitting diodes: Breaking the fundamental bottleneck of deep ultraviolet light sources," *Scientific Reports*, vol. 5, p. 8332, 2015.
- [55] M. Nami and D. Feezell, "Optical properties of Ag-coated GaN/InGaN axial and core–shell nanowire light-emitting diodes," *Journal of Optics*, vol. 17, no. 2, p. 025004, 2015.
- [56] L. C. Chuang, F. G. Sedgwick, R. Chen, W. S. Ko, M. Moewe, K. W. Ng, T. T. Tran, and C. Chang-Hasnain, "GaAs-based nanoneedle light emitting diode and avalanche photodiode monolithically integrated on a silicon substrate," *Nano Lett*, vol. 11, no. 2, pp. 385–390, 2011.
- [57] A. L. Bavencove, D. Salomon, M. Lafossas, B. Martin, A. Dussaigne, F. Levy, B. Andre, P. Ferret, C. Durand, J. Eymery, L. Dang, and P. Gilet, "Light emitting diodes based on GaN core/shell wires grown by MOVPE on n-type Si substrate," *Electronics Letters*, vol. 47, no. 13, pp. 765–766, 2011.
- [58] H. M. Kim, Y. H. Cho, H. Lee, S. I. Kim, S. R. Ryu, D. Y. Kim, T. W. Kang, and K. S. Chung, "High-brightness light emitting diodes using dislocation-free indium gallium nitride/gallium nitride multiquantum-well nanorod arrays," *Nano Letters*, vol. 4, no. 6, pp. 1059–1062, 2004.
- [59] S. Wang, X. Yan, X. Zhang, J. Li, and X. Ren, "Axially connected nanowire core-shell p-n junctions: a composite structure for high-efficiency solar cells," *Nanoscale Res Lett*, vol. 10, no. 1, p. 22, 2015.
- [60] Y. Yu, L. Huang, and L. Cao, "Semiconductor solar superabsorbers," *Scientific Reports*, vol. 4, p. 4107, 2014.
- [61] W. Wang, S. Wu, R. J. Knize, K. Reinhardt, Y. Lu, and S. Chen, "Enhanced photon absorption and carrier generation in nanowire solar cells," *Opt Express*, vol. 20, no. 4, pp. 3733–3743, 2012.
- [62] M. D. Kelzenberg, S. W. Boettcher, J. A. Petykiewicz, D. B. Turner-Evans, M. C. Putnam, E. L. Warren, J. M. Spurgeon, R. M. Briggs, N. S. Lewis, and H. A. Atwater, "Enhanced absorption and carrier collection in Si wire arrays for photovoltaic applications," *Nature Materials*, vol. 9, no. 3, pp. 239–244, 2010.
- [63] E. C. Garnett and P. Yang, "Silicon nanowire radial p-n junction solar cells," *Journal of the American Chemical Society*, vol. 130, no. 29, pp. 9224–9225, 2008.
- [64] L. Tsakalakos, J. Balch, J. Fronheiser, B. A. Korevaar, O. Sulima, and J. Rand, "Silicon nanowire solar cells," *Applied Physics Letters*, vol. 91, no. 23, p. 233117, 2007.
- [65] B. Tian, X. Zheng, T. J. Kempa, Y. Fang, N. Yu, G. Yu, J. Huang, and C. M. Lieber, "Coaxial silicon nanowires as solar cells and nanoelectronic power sources," *Nature*, vol. 449, no. 7164, pp. 885–889, 2007.
- [66] S. Chen, L. You, W. Zhang, X. Yang, H. Li, L. Zhang, Z. Wang, and X. Xie, "Dark counts of superconducting nanowire single-photon detector under illumination," *Opt Express*, vol. 23, no. 8, p. 10786, 2015.
- [67] A. de Luna Bugallo, M. Tchernycheva, G. Jacopin, L. Rigutti, F. H. Julien, S.-T. Chou, Y.-T. Lin, P.-H. Tseng, and L.-W. Tu, "Visible-blind photodetector based on p–i–n junction GaN nanowire ensembles," *Nanotechnology*, vol. 21, no. 31, p. 315201, 2010.

- [68] H. Pettersson, J. Trägårdh, A. I. Persson, L. Landin, D. Hessman, and L. Samuelson, “Infrared Photodetectors in Heterostructure Nanowires,” *Nano Letters*, vol. 6, no. 2, pp. 229–232, 2006.
- [69] H. Kind, H. Yan, B. Messer, M. Law, and P. Yang, “Nanowire Ultraviolet Photodetectors and Optical Switches,” *Adv. Mater.*, vol. 14, no. 2, pp. 158–160, 2002.
- [70] S. Liang, H. Sheng, Y. Liu, Z. Huo, Y. Lu, and H. Shen, “ZnO Schottky ultraviolet photodetectors,” *Journal of Crystal Growth*, vol. 225, no. 2-4, pp. 110–113, 2001.
- [71] S. Grego, K. H. Gilchrist, J.-Y. Kim, M.-K. Kwon, and M. S. Islam, “Nanowire-based devices combining light guiding and photodetection,” *Appl. Phys. A*, vol. 105, no. 2, pp. 311–316, 2011.
- [72] R. F. Oulton, V. J. Sorger, D. A. Genov, D. F. P. Pile, and X. Zhang, “A hybrid plasmonic waveguide for subwavelength confinement and long-range propagation,” *Nature Photonics*, vol. 2, no. 8, pp. 496–500, 2008.
- [73] H. Yamada, M. Shirane, T. Chu, H. Yokoyama, S. Ishida, and Y. Arakawa, “Nonlinear-Optic Silicon-Nanowire Waveguides,” *Japanese Journal of Applied Physics*, vol. 44, no. 9A, pp. 6541–6545, 2005.
- [74] D. J. Sirbuly, M. Law, P. Pauzauskie, H. Yan, A. V. Maslov, K. Knutsen, C. Z. Ning, R. J. Saykally, and P. Yang, “Optical routing and sensing with nanowire assemblies,” *Proceedings of the National Academy of Sciences*, vol. 102, no. 22, pp. 7800–7805, 2005.
- [75] S. Chandrasekhar, J. C. Campbell, A. G. Dentai, and G. J. Qua, “Monolithic integrated waveguide photodetector,” *Electronics Letters*, vol. 23, no. 10, pp. 501–502, 1987.
- [76] A. Zhang, H. Kim, J. Cheng, and Y. H. Lo, “Ultrahigh responsivity visible and infrared detection using silicon nanowire phototransistors,” *Nano Lett.*, vol. 10, no. 6, pp. 2117–2120, 2010.
- [77] H. W. Seo, L. W. Tu, Q. Y. Chen, C. Y. Ho, Y. T. Lin, K. L. Wu, D. J. Jang, D. P. Norman, and N. J. Ho, “Photogated transistor of III-nitride nanorods,” *Applied Physics Letters*, vol. 96, no. 10, p. 101114, 2010.
- [78] A. Persano, M. De Giorgi, A. Fiore, R. Cingolani, L. Manna, A. Cola, and R. Krahne, “Photoconduction properties in aligned assemblies of colloidal CdSe/CdS nanorods,” *ACS Nano*, vol. 4, no. 3, pp. 1646–1652, 2010.
- [79] D. Park and K. Yong, “Photoconductivity of vertically aligned ZnO nanoneedle array,” *Journal of Vacuum Science & Technology B*, vol. 26, no. 6, pp. 1933–1936, 2008.
- [80] V. J. Logeeswaran, A. Sarkar, M. S. Islam, N. P. Kobayashi, J. Strazicky, X. Li, W. Wu, S. Mathai, M. R. T. Tan, S. Y. Wang, and R. S. Williams, “A 14-ps full width at half maximum high-speed photoconductor fabricated with intersecting InP nanowires on an amorphous surface,” *Appl. Phys. A*, vol. 91, no. 1, pp. 1–5, 2008.
- [81] F. Patolsky and C. M. Lieber, “Nanowire nanosensors,” *Materials today*, vol. 8, no. 4, pp. 20–28, 2005.
- [82] F. Qian, Y. Li, S. Gradečak, H.-G. Park, Y. Dong, Y. Ding, Z. L. Wang, and C. M. Lieber, “Multi-quantum-well nanowire heterostructures for wavelength-controlled lasers,” *Nature materials*, vol. 7, no. 9, pp. 701–706, 2008.
- [83] J. C. Johnson, H. Yan, P. Yang, and R. J. Saykally, “Optical cavity effects in ZnO nanowire lasers and waveguides,” *The Journal of Physical Chemistry B*, vol. 107, no. 34, pp. 8816–8828, 2003.
- [84] Y. Y. Wu, H. Q. Yan, M. Huang, B. Messer, J. H. Song, and P. D. Yang, “Inorganic semiconductor nanowires: Rational growth, assembly, and novel properties,” *Chemistry-a European Journal*, vol. 8, no. 6, pp. 1261–1268, 2002.

- [85] B. Ganjipour, S. Sepehri, A. W. Dey, O. Tizno, B. Mattias Borg, K. A. Dick, L. Samuelson, L. E. Wernersson, and C. Thelander, “Electrical properties of GaSb/InAsSb core/shell nanowires,” *Nanotechnology*, vol. 25, no. 42, p. 425201, 2014.
- [86] K. Storm, F. Halvardsson, M. Heurlin, D. Lindgren, A. Gustafsson, P. M. Wu, B. Monemar, and L. Samuelson, “Spatially resolved Hall effect measurement in a single semiconductor nanowire,” *Nat Nanotechnol*, vol. 7, no. 11, pp. 718–722, 2012.
- [87] C. Thelander, L. E. FrobergFroberg, C. Rehnstedt, L. Samuelson, and L.-E. Wernersson, “Vertical enhancement-mode InAs nanowire field-effect transistor with 50-nm wrap gate,” *Electron Device Letters, IEEE*, vol. 29, no. 3, pp. 206–208, 2008.
- [88] Z. W. Pan, Z. R. Dai, and Z. L. Wang, “Nanobelts of semiconducting oxides,” *Science*, vol. 291, no. 5510, pp. 1947–1949, 2001.
- [89] Z. L. Wang and J. Song, “Piezoelectric nanogenerators based on zinc oxide nanowire arrays,” *Science*, vol. 312, no. 5771, pp. 242–246, 2006.
- [90] Z. L. Wang, *Nanowires and Nanobelts: Materials, Properties and Devices. Volume 1: Metal and Semiconductor Nanowires*. Springer Science & Business Media, 2013.
- [91] J. Bae, M. K. Song, Y. J. Park, J. M. Kim, M. Liu, and Z. L. Wang, “Fiber supercapacitors made of nanowire-fiber hybrid structures for wearable/flexible energy storage,” *Angewandte Chemie International Edition*, vol. 50, no. 7, pp. 1683–1687, 2011.
- [92] X. Wang, J. Song, J. Liu, and Z. L. Wang, “Direct-current nanogenerator driven by ultrasonic waves,” *Science*, vol. 316, no. 5821, pp. 102–105, 2007.
- [93] X. Zhao, Y. Ando, Y. Liu, M. Jinno, and T. Suzuki, “Carbon nanowire made of a long linear carbon chain inserted inside a multiwalled carbon nanotube,” *Physical review letters*, vol. 90, no. 18, p. 187401, 2003.
- [94] A. Das, J. Heo, M. Jankowski, W. Guo, L. Zhang, H. Deng, and P. Bhattacharya, “Room Temperature Ultralow Threshold GaN Nanowire Polariton Laser,” *Physical Review Letters*, vol. 107, no. 6, 2011.
- [95] J. X. Ding, J. A. Zapien, W. W. Chen, Y. Lifshitz, S. T. Lee, and X. M. Meng, “Lasing in ZnS nanowires grown on anodic aluminum oxide templates,” *Applied Physics Letters*, vol. 85, no. 12, pp. 2361–2363, 2004.
- [96] B. Xiang, H. Zhang, G. Li, F. Yang, F. Su, R. Wang, J. Xu, G. Lu, X. Sun, Q. Zhao, *et al.*, “Green-light-emitting znse nanowires fabricated via vapor phase growth,” *Applied Physics Letters*, vol. 82, no. 19, pp. 3330–3332, 2003.
- [97] H. J. Joyce, Q. Gao, H. H. Tan, C. Jagadish, Y. Kim, X. Zhang, Y. N. Guo, and J. Zou, “Twin-free uniform epitaxial GaAs nanowires grown by a two-temperature process,” *Nano Letters*, vol. 7, no. 4, pp. 921–926, 2007.
- [98] J. Zhao, X. Liu, W. Qiu, Y. Ma, Y. Huang, J.-X. Wang, K. Qiang, and J.-Q. Pan, “Surface-plasmon-polariton whispering-gallery mode analysis of the graphene monolayer coated InGaAs nanowire cavity,” *Optics Express*, vol. 22, no. 5, pp. 5754–5761, 2014.
- [99] A. Pan, H. Yang, R. Yu, and B. Zou, “Fabrication and photoluminescence of high-quality ternary cdsse nanowires and nanoribbons,” *Nanotechnology*, vol. 17, no. 4, p. 1083, 2006.
- [100] K. H. Li, LiuX, WangQ, ZhaoS, and MiZ, “Ultralow-threshold electrically injected AlGaN nanowire ultraviolet lasers on Si operating at low temperature,” *Nat Nano*, vol. advance online publication, 2015.
- [101] R. Wang, X. Liu, I. Shih, and Z. Mi, “High efficiency, full-color AlInGaN quaternary nanowire light emitting diodes with spontaneous core-shell structures on Si,” *Applied Physics Letters*, vol. 106, no. 26, p. 261104, 2015.

- [102] K. Peng, P. Parkinson, L. Fu, Q. Gao, N. Jiang, Y.-N. Guo, F. Wang, H. J. Joyce, J. L. Boland, M. B. Johnston, H. H. Tan, and C. Jagadish, "Single GaAs/AlGaAs nanowire photoconductive terahertz detectors," in *Optoelectronic and Microelectronic Materials & Devices (COMMAD), 2014 Conference on*, pp. 221–222, 2014.
- [103] W. Wei, Y. Liu, X. Zhang, Z. Wang, and X. Ren, "Evanescent-wave pumped room-temperature single-mode GaAs/AlGaAs core-shell nanowire lasers," *Applied Physics Letters*, vol. 104, no. 22, p. 223103, 2014.
- [104] R. Chen, T.-T. D. Tran, K. W. Ng, W. S. Ko, L. C. Chuang, F. G. Sedgwick, and C. Chang-Hasnain, "Nanolasers grown on silicon," *Nature Photonics*, vol. 5, no. 3, pp. 170–175, 2011.
- [105] G. Zhang, Z. Li, X. Yuan, F. Wang, L. Fu, Z. Zhuang, F.-F. Ren, B. Liu, R. Zhang, and H. H. Tan, "Single nanowire green InGaN/GaN light emitting diodes," *Nanotechnology*, vol. 27, no. 43, p. 435205, 2016.
- [106] "glō-USA, Inc. Sunnyvale, CA, led technology description." <http://www.glo.se/technology.html>. Accessed: 2017-06-10.
- [107] Y. Huang, X. Duan, Y. Cui, and C. M. Lieber, "Gallium nitride nanowire nanodevices," *Nano Letters*, vol. 2, no. 2, pp. 101–104, 2002.
- [108] M. Law, J. Goldberger, and P. D. Yang, "Semiconductor nanowires and nanotubes," *Annual Review of Materials Research*, vol. 34, pp. 83–122, 2004.
- [109] J. Motohisa, J. Noborisaka, J. Takeda, M. Inari, and T. Fukui, "Catalyst-free selective-area movpe of semiconductor nanowires on (111) b oriented substrates," *Journal of Crystal Growth*, vol. 272, no. 1, pp. 180–185, 2004.
- [110] R. Wagner and W. Ellis, "Vapor-liquid-solid mechanism of single crystal growth," *Applied Physics Letters*, vol. 4, no. 5, pp. 89–90, 1964.
- [111] E. Givargizov, "Fundamental aspects of vls growth," *Journal of Crystal Growth*, vol. 31, pp. 20–30, 1975.
- [112] Y. Cui, L. J. Lauhon, M. S. Gudiksen, J. Wang, and C. M. Lieber, "Diameter-controlled synthesis of single-crystal silicon nanowires," *Applied Physics Letters*, vol. 78, no. 15, pp. 2214–2216, 2001.
- [113] H. L. Zhou, T. B. Hoang, D. L. Dheeraj, A. T. van Helvoort, L. Liu, J. C. Harmand, B. O. Fimland, and H. Weman, "Wurtzite GaAs/AlGaAs core-shell nanowires grown by molecular beam epitaxy," *Nanotechnology*, vol. 20, no. 41, p. 415701, 2009.
- [114] C. Colombo, D. Spirkoska, M. Frimmer, G. Abstreiter, and A. F. i Morral, "Ga-assisted catalyst-free growth mechanism of gaas nanowires by molecular beam epitaxy," *Physical Review B*, vol. 77, no. 15, p. 155326, 2008.
- [115] D. Ercolani, F. Rossi, A. Li, S. Roddaro, V. Grillo, G. Salviati, F. Beltram, and L. Sorba, "Inas/insb nanowire heterostructures grown by chemical beam epitaxy," *Nanotechnology*, vol. 20, no. 50, p. 505605, 2009.
- [116] J. Noborisaka, J. Motohisa, S. Hara, and T. Fukui, "Fabrication and characterization of free-standing GaAs/AlGaAs core-shell nanowires and AlGaAs nanotubes by using selective-area metalorganic vapor phase epitaxy," *Applied Physics Letters*, vol. 87, no. 9, pp. –, 2005.
- [117] P. Paiano, P. Prete, N. Lovergne, and A. Mancini, "Size and shape control of gaas nanowires grown by metalorganic vapor phase epitaxy using tertiarybutylarsine," *Journal of applied physics*, vol. 100, no. 9, p. 094305, 2006.
- [118] Q. Wan, Q. Li, Y. Chen, T.-H. Wang, X. He, J. Li, and C. Lin, "Fabrication and ethanol sensing characteristics of zno nanowire gas sensors," *Applied Physics Letters*, vol. 84, no. 18, pp. 3654–3656, 2004.

- [119] Z. Wang and B. Nabet, "Nanowire Optoelectronics," *Nanophotonics*, vol. 4, no. 1, 2015.
- [120] N. S. Kapany and J. J. Burke, "Optical Waveguides (Academic, New York, 1972)," *Chap*, vol. 3, pp. 73–80.
- [121] K. T. Fountaine, W. S. Whitney, and H. A. Atwater, "Resonant absorption in semiconductor nanowires and nanowire arrays: Relating leaky waveguide modes to Bloch photonic crystal modes," *Journal of Applied Physics*, vol. 116, no. 15, pp. –, 2014.
- [122] A. F. Oskooi, D. Roundy, M. Ibanescu, P. Bermel, J. D. Joannopoulos, and S. G. Johnson, "Meep: A flexible free-software package for electromagnetic simulations by the FDTD method," *Computer Physics Communications*, vol. 181, no. 3, pp. 687–702, 2010.
- [123] M. A. Zimmler, J. Bao, F. Capasso, S. Muller, and C. Ronning, "Laser action in nanowires: Observation of the transition from amplified spontaneous emission to laser oscillation," *Applied Physics Letters*, vol. 93, no. 5, p. 051101, 2008.
- [124] M. H. Huang, S. Mao, H. Feick, H. Yan, Y. Wu, H. Kind, E. Weber, R. Russo, and P. Yang, "Room-temperature ultraviolet nanowire nanolasers," *science*, vol. 292, no. 5523, pp. 1897–1899, 2001.
- [125] C. Czekalla, T. Nobis, A. Rahm, B. Cao, J. Zúñiga Pérez, C. Sturm, R. Schmidt Grund, M. Lorenz, and M. Grundmann, "Whispering gallery modes in zinc oxide micro-and nanowires," *physica status solidi (b)*, vol. 247, no. 6, pp. 1282–1293, 2010.
- [126] D. J. Gargas, M. E. Toimil-Molares, and P. Yang, "Imaging single ZnO vertical nanowire laser cavities using UV-laser scanning confocal microscopy," *Journal of the American Chemical Society*, vol. 131, no. 6, pp. 2125–2127, 2009.
- [127] J. Fallert, F. Stelzl, H. Zhou, A. Reiser, K. Thonke, R. Sauer, C. Klingshirn, and H. Kalt, "Lasing dynamics in single ZnO nanorods," *Opt Express*, vol. 16, no. 2, pp. 1125–1131, 2008.
- [128] J. C. Johnson, H.-J. Choi, K. P. Knutsen, R. D. Schaller, P. Yang, and R. J. Saykally, "Single gallium nitride nanowire lasers," *Nat Mater*, vol. 1, no. 2, pp. 106–110, 2002.
- [129] T. Nobis, E. M. Kaidashev, A. Rahm, M. Lorenz, and M. Grundmann, "Whispering gallery modes in nanosized dielectric resonators with hexagonal cross section," *Physical Review Letters*, vol. 93, no. 10, p. 103903, 2004.
- [130] J. Wiersig, "Hexagonal dielectric resonators and microcrystal lasers," *Physical Review A*, vol. 67, no. 2, p. 023807, 2003.
- [131] S.-K. Kim, X. Zhang, D. J. Hill, K.-D. Song, J.-S. Park, H.-G. Park, and J. F. Cahoon, "Doubling Absorption in Nanowire Solar Cells with Dielectric Shell Optical Antennas," *Nano Letters*, 2014.
- [132] X. Zhang, X.-H. Sun, and L.-D. Jiang, "Absorption enhancement using nanoneedle array for solar cell," *Applied Physics Letters*, vol. 103, no. 21, p. 211110, 2013.
- [133] Z. Wang, M. Currie, P. Dianat, G. Konica, P. Prete, N. Lovergne, and B. Nabet, "On Dimensional Dependence of Interaction of Light and Nano Structures," in *Frontiers in Optics*, (Orlando, FL), Optical Society of America, 2013.
- [134] B. H. Le, S. R. Zhao, N. H. Tran, and Z. T. Mi, "Electrically injected near-infrared light emission from single InN nanowire p-i-n diode," *Applied Physics Letters*, vol. 105, no. 23, p. 231124, 2014.
- [135] G. Grzela, R. Paniagua-Domínguez, T. Barten, Y. Fontana, J. A. Sánchez-Gil, and J. Gómez Rivas, "Nanowire antenna emission," *Nano Letters*, vol. 12, no. 11, pp. 5481–5486, 2012.

- [136] A. V. Maslov and C. Z. Ning, "Reflection of guided modes in a semiconductor nanowire laser," *Applied Physics Letters*, vol. 83, no. 6, pp. 1237–1239, 2003.
- [137] B. Hua, J. Motohisa, Y. Ding, S. Hara, and T. Fukui, "Characterization of Fabry-Pérot microcavity modes in GaAs nanowires fabricated by selective-area metal organic vapor phase epitaxy," *Applied Physics Letters*, vol. 91, no. 13, pp. –, 2007.
- [138] D. Saxena, F. Wang, Q. Gao, S. Mokkapati, H. H. Tan, and C. Jagadish, "Mode Profiling of Semiconductor Nanowire Lasers," *Nano Letters*, 2015.
- [139] S. Arab, P. D. Anderson, M. Yao, C. Zhou, P. D. Dapkus, M. L. Povinelli, and S. B. Cronin, "Enhanced Fabry-Perot resonance in GaAs nanowires through local field enhancement and surface passivation," *Nano Research*, vol. 7, no. 8, pp. 1146–1153, 2014.
- [140] D. M. Sullivan, *Electromagnetic simulation using the FDTD method*. John Wiley & Sons, 2013.
- [141] A. Taflove and S. C. Hagness, *Computational electrodynamics*. Artech house, 2005.
- [142] J. D. Jackson and R. F. Fox, "Classical electrodynamics," *American Journal of Physics*, vol. 67, no. 9, pp. 841–842, 1999.
- [143] J. D. Joannopoulos, S. G. Johnson, J. N. Winn, and R. D. Meade, *Photonic crystals: molding the flow of light*. Princeton university press, 2011.
- [144] A.-L. Henneghien, B. Gayral, Y. Désières, and J.-M. Gérard, "Simulation of waveguiding and emitting properties of semiconductor nanowires with hexagonal or circular sections," *JOSA B*, vol. 26, no. 12, pp. 2396–2403, 2009.
- [145] K.-J. Bathe, *Finite element procedures*. Klaus-Jurgen Bathe, 2006.
- [146] I.-H. Tan, G. Snider, L. Chang, and E. Hu, "A self-consistent solution of schrödinger–poisson equations using a nonuniform mesh," *Journal of applied physics*, vol. 68, no. 8, pp. 4071–4076, 1990.
- [147] B. M. Wong, F. Léonard, Q. Li, and G. T. Wang, "Nanoscale effects on heterojunction electron gases in GaN/AlGaN core/shell nanowires," *Nano Letters*, vol. 11, no. 8, pp. 3074–3079, 2011.
- [148] A. Bertoni, M. Royo, F. Mahawish, and G. Goldoni, "Electron and hole gas in modulation-doped  $GaAs/Al_{1-x}Ga_xAs$  radial heterojunctions," *Physical Review B*, vol. 84, no. 20, 2011.
- [149] S. Birner, T. Zibold, T. Andlauer, T. Kubis, M. Sabathil, A. Trellakis, and P. Vogl, "Nextnano: general purpose 3-d simulations," *IEEE Transactions on Electron Devices*, vol. 54, no. 9, pp. 2137–2142, 2007.
- [150] D. Wolf, H. Lichte, G. Pozzi, P. Prete, and N. Lovergne, "Electron holographic tomography for mapping the three-dimensional distribution of electrostatic potential in III-V semiconductor nanowires," *Applied Physics Letters*, vol. 98, no. 26, pp. 264103–264103–3, 2011.
- [151] L. Asryan and R. Suris, "Theory of threshold characteristics of semiconductor quantum dot lasers," *Semiconductors*, vol. 38, no. 1, pp. 1–22, 2004.
- [152] D. J. Bergman and M. I. Stockman, "Surface Plasmon Amplification by Stimulated Emission of Radiation: Quantum Generation of Coherent Surface Plasmons in Nanosystems," *Physical Review Letters*, vol. 90, no. 2, p. 027402, 2003.
- [153] K. Montazeri, Z. Wang, and B. Nabet, "Plasmonic effect of low-dimensional electron gas in core-shell nanowires," in *Frontiers in Optics*, pp. JTh2A–6, Optical Society of America, 2016.
- [154] X. Zhang, J. K. Lin, S. Wickramanayaka, S. Zhang, R. Weerasekera, R. Dutta, K. F. Chang, K.-J. Chui, H. Y. Li, D. S. Wee Ho, L. Ding, G. Katti, S. Bhattacharya, and D.-L. Kwong, "Heterogeneous 2.5D integration on through silicon interposer," *Applied Physics Reviews*, vol. 2, no. 2, p. 021308, 2015.

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## APPENDIX A

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### TRANSITION RATES

This research project focuses on the dimensional dependence of the absorption behavior in semiconductor when interacting with light. Through time-dependent perturbation theory, we find out the transition rate and Fermis Golden Rule, then based on the light interaction Hamiltonian, time average Poynting vector and matrix element, derive the absorption coefficient for bulk semiconductor (3-dimension), quantum well (2-dimension) and quantum wire (1-dimension) structure. Finally, this report will discuss the partial confinement on the electron in the conduction band without the hole confined in the valence band situation.

The Schrödinger equation:

$$\mathcal{H}\Psi(r, t) = -\frac{\hbar}{i} \frac{\partial}{\partial t} \Psi(r, t) \quad (\text{A.1})$$

The Hamiltonian  $\mathcal{H}$  can be expressed as:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}'(r, t) \quad (\text{A.2})$$

where  $\mathcal{H}_0$  is the unperturbed part Hamiltonian and is time-independent,  $\mathcal{H}'(r, t)$  is the small perturbation.

The solution to the unperturbed part is assumed known:

$$\begin{aligned}\mathcal{H}_0\Psi_n(r,t) &= -\frac{\hbar}{i}\frac{\partial}{\partial t}\Psi_n(r,t), \\ \frac{dN_p}{dt} &= \Gamma v_g g N_p + \Gamma \beta_{sp} R_{sp} - \frac{N_p}{\tau_p},\end{aligned}\tag{A.3}$$

The time-dependent perturbation is assumed to have the form

$$\mathcal{H} = \begin{cases} \mathcal{H}'(r)e^{-i\omega t} + \mathcal{H}'^+(r)e^{+\omega t}, & t \geq 0 \\ 0, & t < 0 \end{cases}\tag{A.4}$$

Expand the wave function in terms of the unperturbed solution, we find out  $\Psi(r,t)$ :

$$\Psi(r,t) = \sum_n a_n(t) \Phi_n(r) e^{(-iE_n t/\hbar)}\tag{A.5}$$

$|a_n(t)|^2$  gives the probability that the electron is in the state n at time t.

Substituting the expansion for  $\Psi$  into Schrödinger equation and using A.3, we have

$$\sum_n \frac{da_n(t)}{dt} \Psi_n(r) e^{-iE_n t/\hbar} = -\frac{\hbar}{i} \sum_n \mathcal{H}'(r,t) a_n(t) \Phi_n(r) e^{(-iE_n t/\hbar)}\tag{A.6}$$

Taking the inner product with the wave function  $\Phi_m^*(r)$ , and using the orthonormal property,

$$\int d^3r \Phi_m^*(r) \Phi_n(r) = \delta_{mn}\tag{A.7}$$

We find:

$$\frac{da_n(t)}{dt} = -\frac{i}{\hbar} \sum_n a_n(t) \mathcal{H}'_{mn}(t) e^{i\omega_{mn} t}\tag{A.8}$$

where

$$\begin{aligned}
\mathcal{H}'_{mn}(t) &= \langle m | \mathcal{H}'(\mathbf{r}, t) | n \rangle \\
&= \int \Phi^*_m(\mathbf{r}) \mathcal{H}'(\mathbf{r}, t) \Psi_n(\mathbf{r}) d^3r \\
&= \mathcal{H}'_{mn} e^{-i\omega t} + \mathcal{H}'_{mn} e^{+i\omega t}
\end{aligned} \tag{A.9}$$

$$\omega_{mn} = (E_m - E_n)/\hbar \tag{A.10}$$

and the matrix element is:

$$\mathcal{H}'_{mn}(t) = \int \Phi^*_m(\mathbf{r}) \mathcal{H}'(\mathbf{r}, t) \Psi_n(\mathbf{r}) d^3r \tag{A.11}$$

Introducing the perturbation parameter  $\lambda$

$$\mathcal{H} = \mathcal{H}_0 + \lambda \mathcal{H}'(\mathbf{r}, t) \tag{A.12}$$

and letting

$$a_n(t) = a^{(0)}_n + \lambda a^{(1)}_n(t) + \lambda^2 a^{(2)}_n(t) + \dots \tag{A.13}$$

we can take the derivative and set  $\lambda = 1$

$$\begin{aligned}
\frac{da^{(0)}_n(t)}{dt} &= 0 \\
\frac{da^{(1)}_n(t)}{dt} &= -\frac{i}{\hbar} \sum_n a_n^{(0)}(t) \mathcal{H}'_{mn}(t) e^{i\omega_{mn}t} \\
\frac{da^{(2)}_n(t)}{dt} &= -\frac{i}{\hbar} \sum_n a_n^{(1)}(t) \mathcal{H}'_{mn}(t) e^{i\omega_{mn}t}
\end{aligned} \tag{A.14}$$

Thus, the zeroth-order solutions for equation A.14 are constant. Let the electron be at the state  $i$  initially

$$a^{(0)}_i(t=0) = 1; \quad a^{(0)}_m(t) = 0, \quad m \neq i \tag{A.15}$$

We have the zeroth-order solution

$$a^{(0)}_i(t=0) = 1; \quad a^{(0)}_m(t) = 0, \quad m \neq i \tag{A.16}$$

Therefore, the electron stays at the state  $i$  in the absence of any perturbation. The first order solution is

$$\begin{aligned}
\frac{da_n^{(1)}}{dt} &= -\frac{i}{\hbar} \mathcal{H}'_{mn}(t) e^{i\omega_{mn}t} \\
&= -\frac{i}{\hbar} [\mathcal{H}'_{mi} e^{-i(\omega_{mi}-\omega)t} + \mathcal{H}'_{mi} e^{+i(\omega_{mi}-\omega)t}]
\end{aligned} \tag{A.17}$$

If for final state  $m = f$ ; then integrate above equation, we have

$$a_f^{(1)}(t) = -\frac{i}{\hbar} [\mathcal{H}'_{fi} \frac{e^{-i(\omega_{mi}-\omega)t}}{\omega_{fi} - \omega} + \mathcal{H}'^+_{fi} \frac{e^{+i(\omega_{mi}-\omega)t}}{\omega_{fi} + \omega}] \tag{A.18}$$

If we consider the photon energy to be near resonance, either  $\omega \sim \omega_{fi}$  or  $\omega \sim -\omega_{fi}$ , we find the dominant terms:

$$a_f^{(1)}(t) = \frac{4|\mathcal{H}'_{fi}|^2}{\hbar^2} \frac{\sin^2 \frac{t}{2}(\omega_{fi} - \omega)}{(\omega_{fi} - \omega)^2} + \frac{4|\mathcal{H}'_{fi}|^2}{\hbar^2} \frac{\sin^2 \frac{t}{2}(\omega_{fi} + \omega)}{(\omega_{fi} + \omega)^2} \quad (\text{A.19})$$

where the cross-term has been dropped because it is small compared with either of the above two terms.

When the interaction time is long enough, using approximation

$$\frac{\sin^2(\frac{xt}{2})}{x^2} \rightarrow \frac{\pi t}{2} \delta(x) \quad (\text{A.20})$$

Then

$$|a_f^{(1)}(t)|^2 = \frac{2\pi t}{\hbar^2} |\mathcal{H}'_{fi}|^2 \delta(\omega_{fi} - \omega) + \frac{2\pi t}{\hbar^2} |\mathcal{H}'_{fi}|^2 \delta(\omega_{fi} + \omega) \quad (\text{A.21})$$

The transition rate should be, after using the property of

$$\delta(\hbar\omega) = \frac{\delta(w)}{\hbar} \quad (\text{A.22})$$

$$W_{if} = \frac{d|a_f^{(1)}(t)|^2}{dt} \\ \frac{2\pi}{\hbar} |\mathcal{H}'_{fi}|^2 \delta(E_f - E_i - \hbar\omega) + \frac{2\pi}{\hbar} |\mathcal{H}'_{fi}|^2 \delta(E_f - E_i + \hbar\omega) \quad (\text{A.23})$$

where  $E_f = E_i + \hbar\omega$  represents the absorption of a photon by an electron, and  $E_f = E_i - \hbar\omega$

corresponds with the emission of a photon.

$$I_{hm}^{en} = \int_{-\infty}^{\infty} \Phi_n^*(z) g_m(z) dz, \quad (\text{A.24})$$

$$I_{hm}^{en} = \int_{-\infty}^{\infty} \Phi_n^*(z) g_m(z) dz, \quad (\text{A.25})$$

Therefore, the electron stays at the state  $i$  in the absence of any perturbation. The first order solution is

If we consider the photon energy to be near resonance, either or, we find the dominant terms: The absorption coefficient is a strong function of dimensionality. The confining situation of the quantum structure will considerably affect the energy levels, the overlap function of the conduction and valence band envelope function and also the joint optical density of state. Through the derivation of the absorption coefficient, we can observe the interaction between the light and semiconductor. The next questions should address: 1. The simulation data for single nanowire abs

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## APPENDIX B

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### SEMICONDUCTOR LASER MODELING

In this section, we are trying to delve into the mechanics of how an injected current actually results in an optical output in a semiconductor heterojunction laser by providing a systematic derivation of the dc light-current characteristics. First, the rate equation for photon generation and loss in a laser cavity is developed. This shows that only a small portion of the spontaneously generated light contributes to the lasing mode. Most of it comes from the stimulated recombination of carriers. All of the carriers that are stimulated to recombine by light in a certain mode contribute more photons to that same mode. Thus, the stimulated carrier recombination/photon generation process is a gain process. We find the threshold gain for lasing which is the gain necessary to compensate for cavity losses. The threshold current is the current required to reach this gain

For electrons and holes in the active region of a diode laser, only a fraction,  $\eta_i$ , of injected current will contribute to the generation of carriers. We assumed the active regions that are undoped or lightly doped, so that under high injection levels, charge neutrality applies and the electron density equals the hole density (i.e.,  $N = P$  in the active region). Thus, we can greatly simplify our analysis by specifically tracking only the electron density,  $N$ .

We start with the governing equations of carrier density and photon density in the active region which is governed by a dynamic process.

$$\begin{aligned}\frac{dN}{dt} &= \frac{\eta_i I}{qV} - \frac{N}{\tau} - R_{st}, \\ \frac{dN_p}{dt} &= \Gamma v_g g N_p + \Gamma \beta_{sp} R_{sp} - \frac{N_p}{\tau_p},\end{aligned}\tag{B.1}$$

where  $\beta_{sp}$  is the spontaneous emission factor, defined as the percentage of the total spontaneous emission coupled into the lasing mode. And it is just the reciprocal of the number of available optical modes in the bandwidth of the spontaneous emission for uniform coupling to all modes. The  $g$  is Incremental gain per unit length.

The first term of equation 1 is the rate of injected electrons  $G_{gen} = \Gamma_i I / qV$ ,  $\Gamma_i I / q$  is the number of electrons per second being injected into the active region, where  $V$  is the volume of the active region. The rest terms are the rate of recombining of electrons per unit volume in the active region. There are several mechanisms should be considered, including a spontaneous recombination rate,  $R_{sp}$ , a nonradiative recombination rate,  $R_{nr}$ , a carrier leakage rate,  $R_l$  and a net stimulated recombination,  $R_{st}$ , including both stimulated absorption and emission. Which looks like:

$$R_{rec} = R_{sp} + R_{nr} + R_l + R_{st}\tag{B.2}$$

The first three terms on the right refer to the natural or unstimulated carrier decay processes. The fourth one,  $R_{st}$ , require the presence of photon.

The natural decay process can be described by a carrier lifetime,  $\tau$ . In the absence of photon or a generation term, the rate equation for carrier decay is  $dN/dt = -N/\tau$ , where  $N/\tau = R_{sp} + R_{nr} + R_l$ .

The natural decay rate can also be expressed in a power series of the carrier density,  $N$ . We can also rewrite  $R_{rec} = BN^2 + (AN + CN^3) + R_{st}$ . Where  $R_{sp} = BN^2$  and  $R_{nr} + R_l = (AN + CN^3)$ . The coefficient  $B$  is the bimolecular recombination coefficient, and it has a magnitude,  $B \sim 10^{-10} \text{ cm}^3/\text{s}$  for most AlGaAs and InGaAsP alloys of interest.

When a laser is below threshold, in which the gain is insufficient to compensate for cavity losses,

the generated photons do not receive net amplification. The spontaneous photon generation rate per unit volume is exactly equal to the spontaneous electron recombination rate,  $R_{sp}$ , because an electron-hole pair will emit a photon when they recombine radiatively. Under steady-state conditions ( $dN/dt = 0$ ), the generation rate equals the recombination rate with  $R_{st} = 0$ .

$$\frac{\eta_i I}{qV} = R_{sp} + R_{nr} + R_l \quad (\text{B.3})$$

The spontaneously generated optical power,  $P_{sp}$ , is obtained by multiplying the number of photons generated per unit time per unit volume,  $R_{sp}$ , by the energy per photon,  $hv$ , and the volume of the active region,  $V$ .

$$P_{sp} = hvVR_{sp} = \eta_i\eta_r \frac{hv}{q} I \quad (\text{B.4})$$

The main photon generation term above threshold is  $R_{st}$ . Electron-hole pair is stimulated to recombine, another photon is generated. But since the cavity volume occupied by photons,  $V_p$ , is usually larger than the active region volume occupied by electrons,  $V$ , the photon density generation rate will be  $[V/V_p]R_{st}$ , not just  $R_{st}$ . The electron-photon overlap factor,  $[V/V_p]$ , is generally referred to as the confinement factor,  $\Gamma$ .

## B.1 Threshold or Steady-State Gain in Lasers

The cavity loss can be characterized by a photon decay constant or lifetime,  $\tau_p$ , and the gain necessary to overcome losses, and thus reach threshold. By assuming steady-state conditions (i.e.  $dN_p/dt = 0$ ), and solving for this steady-state or threshold gain,  $g_{th}$ , where the generation term equals the recombination term for photons. We assume only a small fraction of the spontaneous emission is coupled into the mode (i.e.  $\beta_{sp}$  is quite small), then the second term can be neglected,

and we have the solution:

$$\Gamma g_{th} = \frac{1}{v_g \tau_p} = < \alpha_i > + \alpha_m \quad (\text{B.5})$$

The product,  $\Gamma g_{th}$ , is referred to as the threshold modal gain because it now represents the net gain required for the mode as a whole, and it is the mode as a whole that experiences the cavity loss.  $< \alpha_i >$  is the average internal loss, and  $\alpha_m$  is the mirror loss if we considered an in-plane wave laser.

The optical energy of a nano-cavity laser propagates in a dielectric waveguide mode, which is confined both transversely and laterally as defined by a normalized transverse electric field profile,  $U(x, y)$ . In the axial direction this mode propagates as  $\exp(-j\beta z)$ , where  $\beta$  is the complex propagation constant, which includes any loss or gain. Thus, the time- and space-varying electric field can be written as

$$\xi = \hat{e}_y E_0 U(x, y) e^{j(\omega t - \beta z)} \quad (\text{B.6})$$

where  $\hat{e}_y$  is the unit vector indicating TE polarization and  $E_0$  is the magnitude of the field. The complex propagation constant,  $\beta$ , includes the incremental transverse modal gain,  $< g >_{xy}$  and internal modal loss,  $< \alpha_i >_{xy}$ . If we consider a Fabry-Perot laser with the propagating mode is reflected by end mirrors, and the reflection coefficients are  $r_1$  and  $r_2$ , respectively. In addition, the mean mirror intensity reflection coefficient,  $R = r_1 r_2$ .

Define the mirror loss as  $\alpha_m$

$$\alpha_m \equiv \frac{1}{L} \ln\left(\frac{1}{R}\right) \quad (\text{B.7})$$

The photon decay lifetime is given by,

$$\frac{1}{\tau_p} = \frac{1}{\tau_i} + \frac{1}{\tau_m} = v_g (< \alpha_i > + \alpha_m) \quad (\text{B.8})$$

Thus, we can also write

$$\Gamma g_{th} = <\alpha_i> + \alpha_m = \frac{1}{v_g \tau_p} \quad (\text{B.9})$$

## B.2 Threshold Current and Output Power

We construct together a below-threshold and an above-threshold characteristic to illustrate the output power versus input current for a normal diode laser. The first step is to use the below-threshold steady-state carrier rate equation,

$$\frac{\eta_i I_{th}}{qV} = (R_{sp} + R_{nr} + R_l)_{th} = \frac{N_{th}}{\tau} \quad (\text{B.10})$$

Then, recognizing that  $(R_{sp} + R_{nr} + R_l) = AN + BN^2 + CN^3$  depends monotonically on  $N$ , we observe from eq 2.34 that above threshold  $(R_{sp} + R_{nr} + R_l)$  will also clamp at its threshold value, given by Eq 2.35. Thus, we can substitute Eq 2.35 into the carrier rate equation, eq 2.16 to obtain a new above threshold carrier rate equations,

$$\frac{dN}{dt} = \eta_i \frac{(I - I_{th})}{qV} - v_g g N_p, \quad (I > I_{th}) \quad (\text{B.11})$$

We also calculate a steady-state photon density above threshold where  $g = g_{th}$ ,

$$N_p = \frac{\eta_i (I - I_{th})}{qv_g g_{th} V} \quad (\text{steady state}) \quad (\text{B.12})$$

To obtain the power out, we first construct the stored optical energy in the cavity,  $E_{os}$ , by multiplying the photon density,  $N_p$ , by the energy per photon,  $h\nu$ , and the cavity volume,  $V_p$ . That is  $E_{os} = N_p h\nu V_p$ . Then, we multiply this by the energy loss rate through the mirrors,  $v_g \alpha_m = \frac{1}{\tau_m}$ , to get the

optical power output from the mirrors,

$$P_0 = v_g \alpha_m N_p h v V_p \quad (\text{B.13})$$

Substituting from , and using  $\Gamma = V/V_p$ ,

$$P_0 = \eta_i \left( \frac{\alpha_m}{\langle \alpha_i \rangle + \alpha_m} \right) \frac{h v}{q} (I - I_{th}), \quad (I > I_{th}) \quad (\text{B.14})$$

For the output power below-threshold ( $I < I_{th}$ ) can be approximated by neglecting the stimulated emission term and solving for  $N_p$  under steady-state conditions.

$$N_p = \Gamma \beta_{sp} R_{sp} \tau p \quad (I < I_{th}) \quad (\text{B.15})$$

and

$$P_0(I < I_{th}) = \eta_r \eta_i \left( \frac{\alpha_m}{\langle \alpha_i \rangle + \alpha_m} \right) \frac{h v}{q} \beta_{sp} I, \quad (\text{B.16})$$

We can get the threshold carrier density

$$N_{th} = N_{tr} e^{g_{th}/g_0 N} = N_{tr} e^{(\langle \alpha_i \rangle + \alpha_m)/\Gamma g_0 N} \quad (\text{B.17})$$

Using the polynomial fit for the recombination rates, and recognizing that for the best laser material the recombination at threshold is dominated by spontaneous recombination, we have,  $I_{th} \cong BN_{th}^2 qV/\eta_i$ , Thus

$$I_{th} \cong \frac{qVBN_{th}^2}{\eta_i} e^{(\langle \alpha_i \rangle + \alpha_m)/\Gamma g_0 N} \quad (\text{B.18})$$

where for most  $III - V$  materials the bimolecular recombination coefficient,  $B \sim 10^{-10} cm^3/s$ .

For a multiple quantum-well (MQW) lasers, we have to multiply the single-well confinement factor,  $\Gamma_1$ , and volume,  $V_1$ , by the number of wells,  $N_w$ .

$$I_{thMQW} \cong \frac{qN_wV_1BN_{tr}^2}{\eta_i} e^{2(\langle\alpha_i\rangle + \alpha_m)/N_w\Gamma_1 g_0 N} \quad (\text{B.19})$$

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## APPENDIX C

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### MEEP SIMULATION CODE

#### C.1 Cylindrical Core-Shell Nanowire

```

1 ; By Zhihuan Wang , 06-27-2013
2 ; Calculating 1D cylindrical GaAs/AlGaAs core-shell nanowire excitation
   mode using cylindrical coordinates.
3
4 ;%%% length unit %%%
5 ; fundamental length unit in meep is um
6 ;(define nm 0.001)      ; nano-meter unit
7 ;(define um 1)          ; micro-meter unit
8
9 ;-----Parameter Setup-----
10 (define-param nc 3.4) ; index of nanowire core
11 (define-param ns 3.1349) ; index of nanowire shell
12 (define-param w 0) ; width of nanowire
13
14 (define-param r 1.1) ; radius of core
15 (define-param rtotal 1.5) ; radius of total (core+shell)
16
17 (define-param pad 0.5) ; padding between waveguide and edge of PML
18 (define-param gap 0.4) ; padding between cylinder and cell edge in XY plane
19 (define-param dpml 1.5) ; thickness of PML

```

```

20
21 ; -----Dimension and size of the computational cell-----
22 (define sxy (* 2 (+ rtotal w pad dpml))) ; cell size in XY plane
23 (set! geometry-lattice (make lattice (size sxy sxy no-size)))
24
25 ; -----Geometric Setup-----
26 (set! geometry (list
27
28     (make cylinder (center 0 0) (height infinity)
29
30     (radius rtotal ) (material (make dielectric (index ns))))
31
32
33     (make cylinder (center 0 0) (height infinity)
34
35     (radius r) (material (make dielectric (index nc)))))))
36
37 ; -----PML layers set up-----
38 (set! pml-layers (list (make pml (thickness dpml))))
39 (set-param! resolution 20)
40
41 ; -----Source set up-----
42 (define-param fcen 0.15) ; pulse center frequency
43 (define-param df 0.1) ; pulse width (in frequency)
44 ;(define-param nfreq 500); number of frequencies at which to compute flux
45
46 (set! sources (list
47
48     (make source
49
50         (src (make gaussian-src (frequency fcen) (fwidth df)))
51
52         (component Ez) (center (+ rtotal 0.5) 0))))
53
54 ; note that the r -> -r mirror symmetry is exploited automatically
55
56 ; -----run meep-----
57
58 (run-sources+ 300

```

```

49          (at-beginning output-epsilon)
50
51      (after-sources (harminv Ez (vector3 (+ rtotal 0.5) fcen df)))
52
53  (run-until (/ 1 fcen) (at-every (/ 1 fcen 20) output-efield-z))

```

snippet/sourcecode/CylindCS.ctl

## C.2 Hexagonal Core-Shell Nanowire

```

1 ; Calculating GaAs/AlGaAs single Hexagon core-shell nanowire excitation mode
2 ; By Zhihuan Wang 07-01-2013
3 ; Will examine the diameter varing from 20 50 90 130 170 210 250 290 330
4 ; Incident light source wavelength is 532 nm fcen=0.1879
5 ;-----Parameter Setup-----
6 (reset-meep)
7 (define-param n 3.4) ; index of waveguide
8 (define-param ns 3.3) ; index of waveguide shell
9
10 (define-param w 0) ; width of waveguide
11 (define-param r 1.65) ; outer radius of ring
12 (define-param l 10) ; length of the nanowire
13 (define-param rc (* 0.4 r)) ; inner radius of ring
14
15 (define-param pad 0.5) ; padding between waveguide and edge of PML
16 (define-param dpml 1) ; thickness of PML
17
18 ;-----Dimension and size of the computational cell-----
19 (define C->L (compose cartesian->lattice vector3))
20 (define sxy (* 2 (+ r w pad dpml))) ; cell size y
21 (define sxz (* 2 (+ l w pad dpml))) ; cell size z
22

```

```

23 ;-----Geometric Setup-----
24 (set! geometry-lattice (make lattice (size sxy sxy sxz)))
25 (set! geometry (append
26   (list
27     (make block (center 0 0) (size (* r (sqrt (/ 4 3))) (* 2 r) 1)
28       (e1 (C->L 1 0)) (e2 (C->L 0 1))
29         (material (make dielectric (index ns))))
30     (make block (center 0 0) (size (* r (sqrt (/ 4 3))) (* 2 r) 1)
31       (e2 ( C->L (/ (sqrt 3) 2) 0.5)) (e1 (C->L -0.5 (/ (sqrt 3) 2) ))
32       (material (make dielectric (index ns))))
33
34     (make block (center 0 0) (size (* r (sqrt (/ 4 3))) (* 2 r) 1)
35       (e2 ( C->L (/ (sqrt 3) 2) -0.5)) (e1 (C->L 0.5 (/ (sqrt 3) 2) ))
36       (material (make dielectric (index ns))))
37         (make block (center 0 0) (size (* rc (sqrt (/ 4 3))) (* 2 rc) 1)
38           (e1 (C->L 1 0)) (e2 (C->L 0 1))
39             (material (make dielectric (index n))))
40           (make block (center 0 0) (size (* rc (sqrt (/ 4 3))) (* 2 rc) 1)
41             (e2 ( C->L (/ (sqrt 3) 2) 0.5)) (e1 (C->L -0.5 (/ (sqrt 3) 2) ))
42             (material (make dielectric (index n))))
43             (make block (center 0 0) (size (* rc (sqrt (/ 4 3))) (* 2 rc) 1)
44               (e2 ( C->L (/ (sqrt 3) 2) -0.5)) (e1 (C->L 0.5 (/ (sqrt 3) 2) ))
45               (material (make dielectric (index n)))))))
46
47 ;-----PML layers set up-----
48 (set! pml-layers (list (make pml (thickness dpml))))
49 (set-param! resolution 10)
50 ;-----Source set up-----
51 (define-param fcen 0.1879) ; pulse center frequency

```

```

52 (define-param df 0.02) ; pulse width (in frequency)
53 (set! sources (list
54   (make source
55     (src (make gaussian-src (frequency fcen) (fwidth df)))
56     (component Ez) (center (+ r 0.1) 0))))
57
58 ; -----run meep-----
59 (run-sources+ 300
60   (at-beginning output-epsilon)
61   (after-sources (harminv Ez (vector3 (+ r 0.1)) fcen df)))
62 (run-until (/ 1 fcen) (at-every (/ 1 fcen 20) output-efield-z
63   output-tot-pwr))

```

snippet/sourcecode/HexCS3D.ctl

---



---

## APPENDIX D

---

### GAIN SPECTRUM AND THRESHOLD CALCULATION MATLAB CODE

```

1 %% gain (Gain Spectral Analysis Method to determin the enhancement factor for
2 % reduced dimensionality
3 % with Approximations for simple geometry and variables)
4 %
5 % Modified for single band transitions and without scattering broadening effect
6 %
7 % Created on 8/25/2014 By Zhihuan Wang (GaAs/AlGaAs core-shell nanowire)
8 % Modified by 11/4/2016
9 clc; close all;
10
11
12 J_eV = 1.60217657e-19; %Joules per eV
13 eV_J = 6.24150934e18; % eV per Joule
14
15 %% Photon energy & system input (variables initiate)
16 E_ph = 1.2:0.01:2;
17 n = 6e18:3e18:3e19;
18 p = 6e18:3e18:3e19; % Hole carrier concentration , Unit [cm^-3]
19
20 k = length(E_ph);
21 len_n = length(n);
22 abs_coef3D = size(k);
23 abs_coef2D = size(k);
24 abs_coef1D = size(k);
25 k0_3D = size(k);
26 gain_3D = size(k, len_n);

```

```

24 gain_2D = size(k, len_n);
25 gain_1D = size(k, len_n);
26 enhance_abs = size(k);
27 sp_rate3D = size(k);
28 sp_rate2D = size(k);
29 sp_rate1D = size(k);
30 enhance_sp = size(k);
31 st_rate3D = size(k);
32 st_rate2D = size(k);
33 st_rate1D = size(k);
34 enhance_st = size(k);

35
36 f_v = size(k, len_n);
37 f_c = size(k, len_n);
38 Fc = size(len_n);
39 Fv = size(len_n);

40
41 maxgain_3D = size(len_n);
42 maxgain_2D = size(len_n);
43 maxgain_1D = size(len_n);

44 %% Refractive index without material dispersion
45 % Uncommented if need dispersion

46 n_r = 3.312; % refractive index without material dispersion

47
48 %% Parameters in MKS units
49 H_j = 6.63e-34;%Plancks constant [J.s]
50 H = 4.14e-15;%Plancks constant [eV.s]
51 H_rj = 1.05e-34;% Reduced Plancks constant [J.s]
52 H_r = 6.58e-16;% Reduced Plancks constant [eV.s]
53 C = 3e10; %speed of light [cm/s]
54 e = 1.6e-19; %elementary charge [C]
55 kB = 1.38*10^-23; % Boltzmann's constant [J/K]
56 T = 300; % room temperature [K]
57 m0 = 9.11e-31; % Electron rest mass [kg]

```

```

58 Eg=1.424; %Energy bandgap for GaAs at 300K [eV]
59 m_e = 0.067*m0; %Electron Effective mass for GaAs[ unitless /m0]
60 m_h = 0.47*m0; %Hole Effective mass for GaAs 3D[ unitless /m0]
61 m_h2D = 0.118*m0; %Hole Effective mass for GaAs 2D[ unitless /m0]
62 m_h1D = 0.027*m0; %Hole Effective mass for GaAs 1D[ unitless /m0]
63 m_hh = 0.50*m0; %heavey hole Effective mass for GaAs[ unitless /m0]
64 m_lh = 0.087*m0; %Light hole Effective mass for GaAs[ unitless /m0]
65 m_r = m_e*m_h/(m_e+m_h); % Reduced effective mass
66 m_r2D = m_e*m_h/(m_e+m_h2D); % Reduced effective mass 2D
67 m_r1D = m_e*m_h/(m_e+m_h1D); % Reduced effective mass 1D
68
69 m0SI = 5.693e-16; %Electron rest mass [kg]
70 m_eSI = 0.067*m0SI; %Electron Effective mass for GaAs[ unitless /m0]
71 m_hSI = 0.47*m0SI; %Hole Effective mass for GaAs 3D[ unitless /m0]
72 m_rSI = m_eSI*m_hSI/(m_eSI+m_hSI); % Reduced effective mass
73
74 m00 = 9.11*10^-28; %Electron rest mass [kg]
75 m_ee = 0.067*m00; %Electron Effective mass for GaAs[ unitless /m0]
76 m_hh = 0.47*m00; %Hole Effective mass for GaAs 3D[ unitless /m0]
77 m_rr = m_ee*m_hh/(m_ee+m_hh); % Reduced effective mass
78 m_rr2D = m_e*m_h/(m_e+m_h2D); % Reduced effective mass 2D
79 m_rr1D = m_e*m_h/(m_e+m_h1D); % Reduced effective mass 1D
80
81 Lx = 50e-8; % 50 A for length [cm]
82 Ly = 50e-8;
83 Lz = 50e-8;
84 Lz3D = 50e-5; % 50000 A for length [cm]
85 Lz2D = 50e-10; % 5000 A for length [cm]
86 Lz1D = 50e-6; % 50 A for length [cm]
87 Lzm = 100e-10;
88 a = 100e-10; %nanowire crosssection [m]
89 b = 100e-10;
90 p_cv = 2.88*10^-18;
91 f_cv = 23; %oscillator strength 3D [eV]

```

```

92 f_cv1D = 230; %oscillator strength 1D [eV]
93 eps_0 = 8.85e-14; % Permittivity of vacuum [F/cm]
94 Nwr = 1/(Lx*Ly); %nanowire density [cm^-2]
95 Ep = 25.7; % Energy parameter [eV]
96 %% quantized energy state for 2D
97 E_e1 = H_rj^2*pi^2/(2*m_e*Lzm^2)*eV_J;
98 E_h1 = H_rj^2*pi^2/(2*m_h*Lzm^2)*eV_J;
99 E_e2 = H_rj^2*pi^2*4/(2*m_e*Lzm^2)*eV_J;
100 E_h2 = H_rj^2*pi^2*4/(2*m_h*Lzm^2)*eV_J;
101 E_e3 = H_rj^2*pi^2*9/(2*m_e*Lzm^2)*eV_J;
102 E_h3 = H_rj^2*pi^2*9/(2*m_h*Lzm^2)*eV_J;
103
104 E_e1h1 = Eg+E_e1+E_h1; %E_h should be negative value.
105 E_e2h2 = Eg+E_e2+E_h2;
106 E_e3h3 = Eg+E_e3+E_h3;
107
108 %% quantized energy state for 1D
109 E_11 = Eg+H_rj^2/(2*m_r)*((pi/a)^2+(pi/b)^2)*eV_J;
110 E_12 = Eg+H_rj^2/(2*m_r)*((pi/a)^2+(pi*2/b)^2)*eV_J;
111 E_22 = Eg+H_rj^2/(2*m_r)*((pi*2/a)^2+(pi*2/b)^2)*eV_J;
112 E_23 = Eg+H_rj^2/(2*m_r)*((pi*2/a)^2+(pi*3/b)^2)*eV_J;
113 E_33 = Eg+H_rj^2/(2*m_r)*((pi*3/a)^2+(pi*3/b)^2)*eV_J;
114
115 %% Fermi distribution
116 Na = 1e11;%acceptor doping concentration
117 Nd = 1e11;%donor doping concentration
118 Nc = 2*(2*pi*m_e*kB*T/H_j^2)^1.5*10^-6;
119 Nv = 2*(2*pi*m_h*kB*T/H_j^2)^1.5*10^-6;
120 for j=1:len_n
121 Fc(j)= kB*T*(log(n(j)./Nc) + 1/sqrt(8)*(n(j)./Nc))*eV_J;
122 Fv(j)= kB*T*(log(p(j)./Nv) + 1/sqrt(8)*(p(j)./Nv))*eV_J;
123 end
124
125 % Check Joyce-Dixon approximation applicable range -1<theta<7

```

```

126 theta = size(len_n);
127 for j=1:len_n
128     theta(j)= log(n(j)/Nc)+2^(-1.5)*(n(j)/Nc);
129 end
130
131 Ec =size(k);
132 Ev =size(k);
133 for j=1:len_n
134     for i=1:k
135         k0_3D(i) = sqrt(2*m_r*((E_ph(i)-Eg)*J_eV)/H_rj^2);
136         Ev(i) = -H_rj.^2*k0_3D(i).^2/(2*m_h);
137         Ec(i) = Eg+H_rj.^2*k0_3D(i).^2/(2*m_e);
138         f_c(i,j) = (1 + exp((-m_r/m_e*(E_ph(i) - Eg) - Fc(j))/(kB*T*eV_J))).^-1;
139         f_v(i,j) = (1 + exp((-m_r/m_h*(Eg - E_ph(i)) + Fv(j))/(kB*T*eV_J))).^-1;
140     end
141 end
142
143 figure;
144 plot(E_ph, f_c, E_ph, f_v, E_ph, f_c-f_v);
145
146 %% Gain Spectrum: Gain=Absorption Coefficent* fermi distribution (g(hw)=a0(hw)[fv(k0)
147 % -fc(k0)])
148
149 %% Without Linewidth Broadening
150 fe = size(k,len_n);
151 for j=1:len_n
152     for i=1:k
153         if E_ph(i)< Eg
154             gain_3D(i,j) = 0;
155         else
156             gain_3D(i,j) = (sqrt(2)*m_r^1.5*(e*eV_J)^2*(1.5*m0*E_p*J_eV/6))/(3*pi*n_r*m0*eps_0*C*
157             H_rj^2*E_ph(i))*(E_ph(i)-Eg)^0.5*(f_c(i,j)-f_v(i,j));
158         end
159     if E_ph(i)< E_e1h1

```

```

158 gain_2D(i,j) = 0;
159 elseif E_e1h1<= E_ph(i)
160 gain_2D(i,j) = (e^2*pi*H_r*(1.5*m0*Ep*J_eV/6)*2)/(3*n_r*eps_0*C*m0^2*E_ph(i))*m_r2D/(H_rj^2*pi*Lz)*(f_c(i,j)-f_v(i,j));
161 end
162
163 if E_ph(i)< E_11
164 gain_1D(i,j) = 0;
165 elseif E_11<= E_ph(i)
166 gain_1D(i,j) = (e^2*pi*H_r*Nwr)/(3*n_r*eps_0*C*m0^2*E_ph(i))*(m0*Ep*10*J_eV/6)*(m_r1D^1.5/(pi*H_rj*m_e*Lx*Ly))*((E_ph(i)-E_11)^-0.5*(f_c(i,j)-f_v(i,j)));
167 end
168
169 maxgain_3D(j)= max(gain_3D(:,j));
170 maxgain_2D(j)= max(gain_2D(:,j));
171 maxgain_1D(j)= max(gain_1D(:,j));
172 enhance_abs(i,j) = gain_2D(i,j)/gain_3D(i,j);
173
174 end
175 end
176
177 %% Plotting the results
178 figure;
179 subplot(2,2,1);
180 plot(E_ph, gain_3D, 'LineWidth',4)
181 title('Gain coefficient versus photon energy for 3D')
182 ylabel('Gain coefficient (/cm)')
183 xlabel('photon energy (eV)')
184 grid on,
185
186 subplot(2,2,2);
187 plot(E_ph, gain_2D, 'LineWidth',4)
188 title('Gain coefficient versus photon energy for 2D')
189 ylabel('Gain coefficient (/cm)')

```

```

190 xlabel ('photon energy (eV)')
191 grid on,
192
193 subplot(2,2,3);
194 plot(E_ph, gain_1D, 'LineWidth',4)
195 title('Gain coefficient versus photon energy for 1D')
196 ylabel ('Gain coefficient (/cm)')
197 xlabel ('photon energy (eV)')
198 grid on,
199
200 subplot(2,2,4);
201 plot(n, maxgain_2D, 'LineWidth',4)
202 title('Maximum gain versus carrier density')
203 ylabel ('Gain coefficient (/cm)')
204 xlabel ('Carrier density (1/cm^2)')
205 grid on,
206 %% Curve fitting in order to find the threshold carrier density
207 % which is nth = 4.533*10^18 (1/cm^3)
208
209 nth = 4.533*10^18; % Unit (1/cm^3)
210 % nth = Ntr*exp(gth/g0)
211
212 %% Fermi distribution for threshold carrier density
213 Fc_th= kB*T*(log(nth/Nc) + 1/sqrt(8)*(nth/Nc))*eV_J;
214 Fv_th= kB*T*(log(nth/Nv) + 1/sqrt(8)*(nth/Nv))*eV_J;
215
216 f_vth = size(k);
217 f_cth = size(k);
218 for i=1:k
219 f_vth(i) = (1 + exp((-m_r/m_h*(E_ph(i) - Eg) + Fv_th)/(kB*T*eV_J))).^-1;
220 f_cth(i) = (1 + exp((-m_r/m_e*(E_ph(i) - Eg) - Fc_th)/(kB*T*eV_J))).^-1;
221 end
222
223 %% Calculating rsp and Rsp based on the threshold carrier density

```

```

224 % Spontaneous Emission Spectrum: sp_rate = Emission Probability * Density of States *
225 % fermi distribution
226
227 for i=1:k
228 if E_ph(i)< Eg
229 sp_rate3D(i) = 0;
230 else
231 sp_rate3D(i) = (n_r*e^2*E_ph(i)*Ep*J_eV/6)/(pi*m0^2*eps_0*C^3*H_r^2)*((2*m_r)^1.5)
232 /(2*pi^2*H_r^3)*((E_ph(i)-Eg)*J_eV)^0.5*(f_cth(i)*(1-f_vth(i)));
233 end
234
235 if E_ph(i)< E_e1h1
236 sp_rate2D(i) = 0;
237 elseif E_e1h1<= E_ph(i)
238 sp_rate2D(i) = (n_r*e^2*E_ph(i)*J_eV*Ep*J_eV/6)/(pi*m0^2*eps_0*C^3*H_r^2)*(m_r2D*2)/(
239 pi*H_r^2*Lz2D)*(f_cth(i)*(1-f_vth(i)));
240 end
241
242 if E_ph(i)< E_11
243 sp_rate1D(i) = 0;
244 elseif E_11<= E_ph(i)
245 sp_rate1D(i) = (n_r*e^2*E_ph(i)*J_eV*Ep*J_eV/6)/(pi*m0^2*eps_0*C^3*H_r^2)*(m_r1D
246 ^1.5/(pi*H_r*m_e*Lz1D*Lz1D))*(E_ph(i)-E_11)^-0.5*(f_cth(i)*(1-f_vth(i)));
247 end
248
249 Rst_3D = trapz(sp_rate3D)';
250 Rst_2D = trapz(sp_rate2D)';
251 Rst_1D = trapz(sp_rate1D)';
252
253 %% Threshold current calculation

```

```

254
255 Jth_3D = e*Lz*Rst_3D ;
256 Jth_2D = e*Lz*Rst_2D ;
257 Jth_1D = e*Lz*Rst_1D ;
258
259 %% Optical Output Power
260
261 P_3D = (Eg+0.0257/2)*Lz*Rst_3D ;
262 P_2D = (Eg+0.0257/2)*Lz*Rst_2D ;
263 P_1D = (Eg+0.0257/2)*Lz*Rst_1D ;
264 enhance_2D = P_2D/P_3D
265 enhance_1D = P_1D/P_3D
266
267 %% Plotting the results
268 figure ;
269 subplot(2,2,1) ;
270 plot(E_ph, sp_rate3D)
271 title('Spontaneous Emission Rate versus photon energy for 3D')
272 ylabel('Spontaneous Emission Rate (/cm)')
273 xlabel('photon energy (eV)')
274 grid on,
275
276 subplot(2,2,2) ;
277 plot(E_ph, sp_rate2D)
278 title('Spontaneous Emission Rate versus photon energy for 2D')
279 ylabel('Spontaneous Emission Rate (/cm)')
280 xlabel('photon energy (eV)')
281 grid on,
282
283 subplot(2,2,3) ;
284 plot(E_ph, sp_rate1D)
285 title('Spontaneous Emission Rate versus photon energy for 1D')
286 ylabel('Spontaneous Emission Rate (/cm)')
287 xlabel('photon energy (eV)')

```

```

288 grid on,
289
290 subplot(2,2,4);
291 barx = [1 2 3];
292 bary = [Jth_3D, Jth_2D, Jth_1D];
293 bar (barx,bary);
294 set(gca,'YScale','log');
295 set(gca,'XTickLabel',{ '3D', '2D', '1D'});
296 for i1=1:numel(bary)
297 text(barx(i1),bary(i1),num2str(bary(i1),'%2.2E'),...
298 'HorizontalAlignment','center',...
299 'VerticalAlignment','bottom')
300 end
301 title('Threshold Current density for different dimensionality')
302 ylabel ('Threshold Current Density (A/cm^2)')
303 xlabel ('Dimensions')
304 grid on,
305
306
307 %% Additional overlapping Plot
308 figure;
309 ax1 = gca;
310 get(ax1,'Position');
311 set(ax1,'XColor','k',...
312 'YColor','b');
313 line(E_ph,sp_rate1D, 'Color','b', 'LineStyle', '-','Marker', '.', 'Parent', ax1, ...
314 'DisplayName', '1D','LineWidth',4)
315 legend show
316 ax2 = axes('Position',get(ax1,'Position'),...
317 'XAxisLocation','bottom',...
318 'YAxisLocation','left',...
319 'Color','none',...
320 'YLim',[0,10*10^4],...
321 'YTick',[1*10^4, 3*10^4, 5*10^4, 7*10^4, 9*10^4],...

```

```

321 'XColor','k',...
322 'YColor','r',...
323 'XTick',[],'XTickLabel',[]);  

324 set(gca, 'YTickLabel', num2str(reshape(get(gca, 'YTick'),[],1), '%.d') );  

325 ylabel ('Spontaneous Emission Rate (/cm.s)')  

326 line(E_ph,sp_rate2D, 'Color', 'r', 'LineStyle', '-','Marker', '.', 'Parent', ax2,'  

   DisplayName', '2D','LineWidth',4)  

327 legend show  

328 ax3 = axes('Position',get(ax1,'Position'),...  

   'XAxisLocation','bottom',...
329 'YAxisLocation','right',...
330 'Color','none',...
331 'YLim',[0,10*10^3],...
332 'YTick',[1*10^3, 3*10^3, 5*10^3, 7*10^3, 9*10^3],...
333 'XColor','k',...
334 'YColor','g',...
335 'XTick',[],'XTickLabel',[]);  

336 line(E_ph,sp_rate3D, 'Color', 'g', 'LineStyle', '-','Marker', '.', 'Parent', ax3,'  

   DisplayName', '3D','LineWidth',4)  

337 legend show  

338 ylabel ('Spontaneous Emission Rate (/cm.s)')  

339 xlabel ('Photon energy (eV)')  

340 xlabh = get(gca,'XLabel');  

341 set(xlabh,'Position',[get(xlabh,'Position') - [0 0.2 0]]);  

342 grid on,

```

snippet/sourcecode/gain1band.m

---

## VITA

### ZHIHUAN WANG

PLACE AND DATE OF BIRTH: Beijing, China — 15 August 1986  
 ADDRESS: 3602 Hamilton St., Apt. 2, Philadelphia, PA, 19104, US  
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### WORK EXPERIENCE

<i>Present - JUN 2015</i>	<b>BROOKHAVEN NATIONAL LABORATORY</b> , Long Island, NY, US <i>Visiting Scientist</i> <ul style="list-style-type: none"> <li>• Performed SEM/TEM imaging of as-grown and dispersed core-shell nanowires in the clean room of center for fundamental nanomaterials.</li> <li>• Developed contacts of dispersed single nanowire by FIB, then characterized the device by I-V, C-V measurement and Photoluminescence spectroscopy.</li> </ul>
<i>Present - MAR 2012</i>	<b>DREXEL UNIVERSITY</b> , Philadelphia, PA, US <i>Graduate Research Fellow</i> <p>The focus of my research is on characterizing the extremely enhanced optical properties of core-shell nanowires and analyzing the fundamental mechanism of such significant enhancement in light absorption, emission and lasing behavior. Specifically optoelectronic characteristics and light-matter interactions of this novel nano-structure are in my interest. Meanwhile, I also participated in writing proposals for research grants from National Science Foundation, and for access permission to center for fundamental nanomaterials at Brookhaven National Lab.</p>
<i>Present - MAR 2012</i>	<b>DREXEL UNIVERSITY</b> , Philadelphia, PA, US <i>Teaching Assistant</i> <p>Involved dynamically in teaching responsibilities, e.g. running lectures, managing labs and carrying recitations and office hours in various courses including Electronic Devices, Analog Devices, Design for Microcontrollers, Digital Systems, Electrical Engineering Lab, Evaluation and Present Experimental Data, Linear and Dynamic Engineering System, and Statistic Analysis of Engineering System, Introduction to Physics.</p>
<i>Aug 2011 - FEB 2011</i>	<b>IM FLASH SINGAPORE LLP.</b> , Singapore <i>(A Joint-Venture of Intel and Micron)</i> <i>Process Integration Engineer</i> <ul style="list-style-type: none"> <li>• Written analyze report for Special Work Requests and Global Conversion to align new process recipes and tools between Singapore and US.</li> <li>• Developed, maintained and improved a process module on an advance NAND Flash Memory including design rules for alternative flows.</li> <li>• Optimized existing process flows and developed creative solutions to meet product requirements.</li> <li>• Extracted, monitored, analyzed and reacted to inline data, param data and probe data to fix yield issues, add process margin and reduce costs.</li> </ul>

## EDUCATION

---

<i>Present -</i>	<b>Drexel University</b> , Philadelphia, PA, US
SEP 2011	Doctor of Philosophy in ELECTRICAL ENGINEERING Research Field: <i>Solid State and Photonic Devices</i> — Advisor: Dr. Bahram NABET GPA: 3.93/4
<i>Dec 2010 -</i>	<b>Nanyang Technological University</b> , Singapore
AUG 2009	Master of Science in ELECTRONICS Thesis: “Numerical Characterization of Nanowire Transistors and Logic Gates with Parametric Variations” — Advisor: Dr. Xing ZHOU GPA: 4.2/5
<i>Jun 2009 -</i>	<b>Huazhong University of Science and Technology</b> , Wuhan, China
SEP 2005	Bachelor of Engineering in COMMUNICATION ENGINEERING Thesis in Chinese: “Simulation of Wireless Streaming Media Distribution with Performance Evaluation” — Advisor: Dr. Xu DU GPA: 82/100

## AWARDS AND CERTIFICATES

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2011-PRESENT	Dean's List for graduate students with an outstanding curriculum, Drexel University
JAN 2016	Allen Rothwarf Endowed Fellowship, Drexel University
OCT 2015	Graduate Student Domestic Travel Grant The Graduate College of Drexel University
SEP 2015	Finalist for Jean Bennett Memorial Student Travel Grant out of 200 applications, The Optical Society (OSA)
APR 2015	Best Poster Award of Drexel IEEE Graduate Forum's 7 <sup>th</sup> Annual Research Poster Symposium
APR 2013	Best Student Poster in Physics, Drexel Research Day
NOV 2010	Best M.S. Dissertation, NTU
AUG 2009	Graduate Fellowship from Minister of Education of Singapore, NTU
MAY 2009	Best Engineering Undergraduate Thesis, Internet Technology and Engineering Research Center at HUST
OCT 2010	GRE(R): 1430 (Q:800;V:630) 94 <sup>th</sup> percentile; AWA: 3.0/6.0

## PUBLICATIONS

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1. Z. Wang, B. Nabet,”Nanowire Optoelectronics” *Nanophotonics*, 4.1 (2015): -. Retrieved 17 Mar. 2016, from doi:10.1515/nanoph-2015-0025.
2. Z. Wang, B. Nabet,”Enhancement of Optoelectronic Properties of Nanowires” Submitted to Physical Review Letter, 2017.
3. K. Montazeri, Z. Wang, B. Nabet,”Plasmonic Effect of Low-Dimensional Electron Gas in Core-Shell Nanowires” in Frontiers in Optics 2017, OSA Technical Digest (online) (Optical Society of America, 2017), paper JTh2A.6.
4. Z. Wang, B. Nabet,”Light and Rate Management in Nanowires” in Frontiers in Optics 2015, OSA Technical Digest (online) (Optical Society of America, 2015), paper FW5C.6.
5. Z. Wang, M. Currie, P. Prete, N. Lovergne, B. Nabet,”Lasing from As Grown GaAs-AlGaAs Core-Shell Nanowires up to Room Temperature” in Frontiers in Optics 2015, OSA Technical Digest (online) (Optical Society of America, 2015), paper LTh2I.4.
6. Z. Wang, M. Currie, P. Prete, N. Lovergne, B. Nabet,”Room Temperature Lasing of GaAs-AlGaAs Core-Shell Nanowires Grown on Silicon Substrate” Accepted in proceeding of: 2<sup>nd</sup> EOS Topical Meeting on Optics at the Nanoscale (ONS15), At Capri, Italy. Sep 17-19, 2015.

7. Z. Wang, M. Currie, P. Dianat, G. Konica, P. Prete, N. Lovergne, et al., "On Dimensional Dependence of Interaction of Light and Nano Structures," In proceeding of: Frontiers in Optics, At Orlando, FL. Oct 10-12, 2013.
8. M. Currie, Z. Wang, P. Dianat, P. Prete, I. Miccoli, N. Lovergne, et al., "Large Light Emission Enhancement in GaAs/AlGaAs CoreShell Nanowires," In proceeding of: International Conference on One-Dimensional Nanomaterials, ICON2013, At Annecy, France. Sep, 2013.
9. Zhou, X., Zhu, G. J., Srikanth, M. K., Lin, S. H., Chen, Z. H., Zhang, J. B., ... & Wang, Z. (2010). Xsim: Benchmark Tests for the Unified DG/GAA MOSFET Compact Model. Proc. Nanotech, 2, 785-788.

## POSTER PRESENTATIONS & PANELS

---

1. Efficiency and Transition Rate Enhancement of Quantum Well and Core-Shell Nanowire Lasers, Drexel IEEE Graduate Forums 9th Annual Research Poster Symposium, March, 2017.
2. A Novel Alternative Infrastructure for Efficient High Volume Computation, Drexel IEEE Graduate Forums 7th Annual Research Poster Symposium, April, 2015.
3. Volumetric Optical Cavity Modes Allow Room Temperature GaAs/AlGaAs Core-Shell Nanowire Lasing, Drexel Research Day, April, 2014 & Nano for Business, Lehigh University, June, 2014.
4. As-grown GaAs/AlGaAs core-shell nanowire lase at room temperature, Drexel IEEE Forum, March, 2014.
5. Strong Photoluminescence Enhancement of Single GaAs/AlGaAs Core-Shell Nanowire, Drexel Research Day, April, 2013.

## LANGUAGES

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CHINESE: Native Proficiency  
 ENGLISH: Full Professional Proficiency  
 FRENCH: Basic Knowledge

## RESEARCH SKILLS

---

Semiconductor Fabrication and Characterization:	Photoluminescence\Electroluminescence Spectroscopy, Scanning\Atomic\Tunneling Microscopy, THz Time-Domain Spectroscopy, Electron Beam Induced Current, Low and High-Temperature Electronic Probing and e-beam Lithography
Computer:	Microsoft Excel, Word, PowerPoint, PHP, MySQL, HTML, MATLAB, MEEP, Python, Adobe Photoshop and Illustrator, Sketchup, LINUX, ubuntu, LATEX

## PROFESSIONAL & ACADEMIC MEMBERSHIP

---

<i>Starting Jun 2015</i>	<b>OSA, Member</b>
<i>Starting Jun 2015</i>	<b>APS, Member</b>
<i>Starting Aug 2013</i>	<b>IEEE, Member</b>

## INTERESTS AND ACTIVITIES

---

<i>Present - AUG 2015</i>	<b>Assistant Operation Officer</b> , Drexel IEEE Graduate (DIG) <ul style="list-style-type: none"> <li>• Served the Graduate IEEE community for contacting companies and academic professors for sponsorship and technical talks.</li> <li>• Organized and served as judge for Drexel IEEE Graduate Forum's 8<sup>th</sup> Annual Research Poster Symposium</li> </ul>
<i>Present - AUG 2015</i>	<b>First Drexel Diversity Council Advisory Board</b> , Student Center for Inclusion and Culture (SCIC) <ul style="list-style-type: none"> <li>• Encouraged open communication and dialogue, collaboration and promotion of inclusive programming on campus.</li> <li>• Created a space where diverse student leaders collaborate and communicate with each other and the SCIC.</li> </ul>

Technology, Open-Source, Programming  
 Paradoxes in Decision Making, Behavioral Finance, Stock  
 Basketball, Traveling, Running

