Study of Nano-scale ITO Top Grating of GaN LED

by

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Acknowledgements

I would like to express my appreciation to Dr. Jin for her advice and insight. She has introduced me to the field of simulation based LED research and I have enjoyed learning a new subject and discovering new things. Thank you for your guidance and critiques; they have been invaluable to me since starting this project.

Abstract

This is an international research collaboration project in which students in Peking University (PKU), Beijing, China and at California Polytechnic State University (Cal Poly) work together. Comprehensive study on ITO nano-gratings analysis is still very novel in this field. We provide a systematic study of nano-scale transmission ITO gratings through the finite difference time domain (FDTD) simulation and find the following novel statements: The total light extraction highly depends on the grating duty cycle. Generally, the optimum duty cycle increases as the grating cell width increases. Adding a nano-scale grating with optimum duty cycle increases LED light extraction efficiency up to 165.67% when compared to a non-grating GaN LED. Therefore, this work provides the guideline for GaN LED ITO nano-grating design.

Introduction

Since the invention of the first high brightness GaN LED by Shuji Nakamura in 1996, production of white LED lighting utilizing GaN material has started. However, the performance for GaN LEDs cannot be specified without the ability to model them. The GaN device models are still being discussed and investigated by many research groups since no one can explain how exactly the GaN LED can emit light efficiently with a lot of defects from device fabrication, which is difficult to avoid for GaN material. Researchers are still working diligently to apply semiconductor theory to GaN LEDs technology.

This project is a collaboration between California Polytechnic State University (Cal Poly) and Peking University (PKU) on gallium nitride (GaN) light emitting diode (LED) research. In this project, we developed novel models for GaN LEDs, and define design rules for those devices. The major goal of the project is to develop a comprehensive GaN LED device model, which can be used to jointly develop, fabricate and test novel GaN LEDs. It is very expensive to fabricate different photonic devices and make direct comparisons. Our device model will provide capabilities for the device selection, and the modification or/and optimization of device design and performance. Last summer (2013), I visited and studied at PKU for 6 weeks. During the visit, I found there is no systematic study of nano-scale ITO grating design in print. Therefore I worked very hard to create a GaN LED simulation model last year, figured out new design rules, and submitted my new results to SPIE Photonic West, San Franccisco, CA, Feb 2014, which was accepted.

A GaN-based LED has a low energy consumption and a longer lifetime, which continues to be proved useful in industries and is gaining popularity in the solid-state electronics and lighting industries [1-2]. LEDs have replaced fluorescent lamp backlighting in cell phones, TVs and monitor displays. The LED is lighting households and businesses due to its minimum power consumption, maximum efficiency, minimum heat generation, and long lifetime [2]. Increasing electroluminescent efficiency and light extraction efficiency improves an LED’s performance characteristics [3]. Our study focuses on increasing the light extraction efficiency by adding nano-scale gratings to the surface of GaN LED devices.

In an LED, light extraction inefficiency is due to the difficulty of light generated within a high-index material to propagate into a surrounding medium of a low-index, usually being air. In general, the efficiency of a LED is limited by the maximum angle that light can escape from the surface as defined by Snell's law. Light can only escape the LED if it approaches the surface within 23° of normal since GaN has a high index of refraction compared to air. Adding a material with an index of refraction between the indices of GaN and air to a LED surface increases the limiting angle [3-7]. Several research groups have used gratings as a method for increasing light output and placed these gratings on the surface and/or bottom of the LED [8-10]. Gratings can vary in the following ways: (1) placing the grating on different

layers within the thin-film LED, (2) varying the density of grating cells on the grating layer, (3) altering the shape of the grating cells, and (4) increasing the symmetry of the photonic crystal grating [9]. However, most publications on transmission gratings are either focused on micro-grating simulations or are micro/nano-grating experiments. We are the first group to present a systemic design simulation on GaN LED nano-ITO grating design.

This paper investigates the light extraction enhancements of surface nano-scale gratings with duty cycles ranging from 0-100% and ITO layer thickness of 78nm and 230nm. Section 2 illustrates and describes the simulation model and discusses the device parameters. Section 3 uses FDTD analysis to compare light extraction efficiency for grated and non-grated models. Section 4 concludes this paper by providing a summary of results.

Requirments

1. Improves light extraction efficiency compared to a conventional LED.
2. Utilizes optimum ITO thickness, grating duty cycle, and grating dimensions.
3. Simulations use FDTD method to obtain accurate light extraction data from CAD models.
4. Deepen understanding of the filling factor's effect on sub-wavelength gratings on GaN LEDs.
5. Draw some meaningful conclusions from the results.

Simulation Model

In this paper, we consider the top transmission grating's effects on GaN LED light extraction efficiency (LEE). We explore different LED layer thicknesses and try different transmission grating patterns. We study the effects that grating patterns and layer thicknesses have on total light transmission across the LED device using the finite difference time domain (FDTD) method. Our simulations allow us to improve the LEE by optimizing the device parameters.

Our device consists of a two-dimensional model of GaN with triangular ITO grating cells arranged in a crystal lattice atop an ITO layer thickness. We use a 10 μm sapphire substrate and define air as the surrounding medium. The LED model shown in Figure 1 consists of an ITO top triangular grating with ITO layer thickness, p-GaN layer, MQWs, n-GaN layer, and a sapphire substrate. Table1 includes the material thicknesses and refractive indices of each layer, all those value are from PKU experimental data.

Our model assumes plane wave incidence and lossless material, with light propagating in the positive z-direction and originating from the MQW region. Our simulations use a field source defined along the center of the MQW region to emit an incident plane wave with 460nm wavelength. The GaN LED grating model shown in Figure2 illustrates the parameters that influence the top grating structure. The ratio of grating width and grating period defines the grating duty cycle, which varies from 0-100%. We simulated three grating width cases: 125nm, 230nm, 460nm and two ITO layer thicknesses: 78nm and 230nm, and keep the grating height equal to the grating width. The ratio of the width of LED device (10.5μm) and the grating period defines the number of triangular ITO grating cells atop the ITO layer. These calculations determine the arrangement of the triangular top gratings for each simulation.

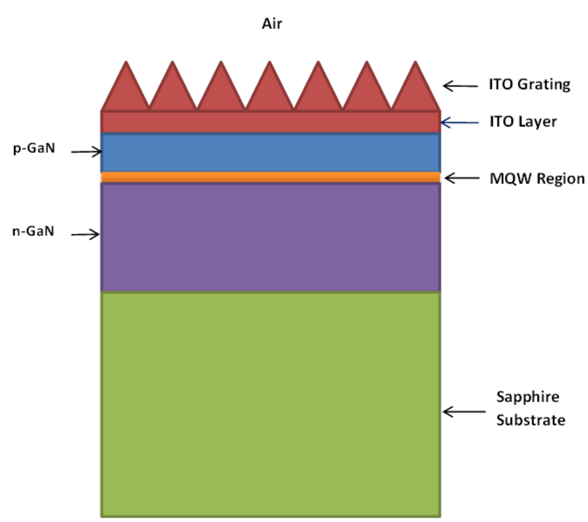

Figure 1: Simulation Model of LED used in the FDTD calculations

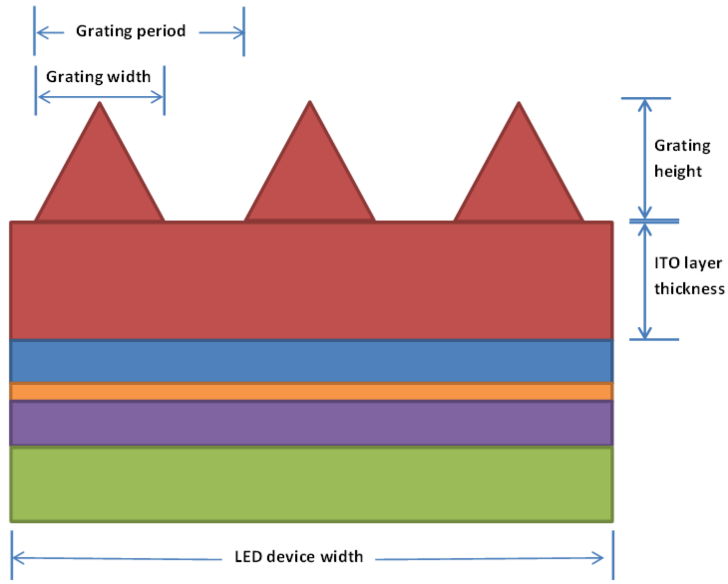

Figure 2: Transmission grating GaN LED model

Table 1: LED material thickness and refractive index

Material	Thickness (µm)	Refractive Index
p-GaN	0.2	2.5
MQWs	0.1	2.6
n-GaN	5	2.5
Sapphire	10	1.78
ITO Layer	0.078 / 0.23	2.1
Air	>10000	1

FTDT Analysis

First, using an ITO layer thickness of 78nm, we analyze the effect the duty cycle of top triangular gratings has on the total light extraction. We increase the duty cycle from 0-100%, 0% duty cycle being the non-grating case, for grating cell widths of 125nm, 230nm and 460nm (suggested by experiment) by varying the grating period from 1250nm to 125 nm, 2300nm to 23onm, and 4600nm to 460nm respectively. Fig.3 depicts the output power of light extracted versus the duty cycle of triangular grating cells for an ITO layer thickness of 78nm. In general, top light emission is preferred over bottom or side light emissions. However, total light emission peaks are not always aligned with top light emission peaks, however they are very close. For a cell width of 125nm, total light extraction improves only in 1-50% duty cycles, shown in Fig.3(a). The greatest light extraction occurs at 30% duty cycle improving total light extraction by 88.75% compared to the non-grating case. Little variation of light intensity occurs between 50-100% duty cycles. For a cell width of 230nm, total light extraction improves between 1-80% duty cycles as shown in Fig.(b). The greatest light extraction occurs at 50% duty cycle improving total light extraction by 136.77% compared to the non-grating case. For a cell width of 460nm, total light extraction improves around 40% and 60-100% duty cycles as shown in Fig3(c). The greatest light extraction occurs at 60% duty cycle improving total light extraction by 96.74% compared to the non-grating case. We notice as the width of the triangular grating cell increases (125nm, 230nm, 460nm), the optimum duty cycle increases (30%, 50%, 60%). For ITO layer thickness of 78nm, a 230nm grating cell width with 50% duty cycle achieves the greatest total light extraction resulting in a 136.77% improvement over the non-grating case.

Next, we use an ITO layer thickness of 230nm and again analyze the effect grating duty cycle has on the amount of light extracted from the device, shown in Fig.4. Similarly, we increase the duty cycle from 0-100% and use 0% duty cycle as the non-grating case. For a cell width of 125nm, 230nm, and 460nm, we see the similar trends: 1) Total light extraction improves between 1-50%, 1-80%, around 40% and 60-100% duty cycles, respectively. 2) The greatest light extraction occurs at 30%, 50%, 70% duty cycle improving total light extraction by 113.01%, 165.7%, 68.01%, respectively, compared to the non-grating case. For ITO layer thickness of 230nm, a 230nm grating cell width with 50% duty cycle achieves the greatest total light extraction resulting in a 165.67% improvement over the non-grating case. Our results show that total light extraction highly depends on the grating duty cycle. Generally, the optimum duty cycle increases as the grating cell width increases. We also demonstrate that implementing a top grating having a full wavelength period and a half wavelength cell width can maximize light extraction efficiency.

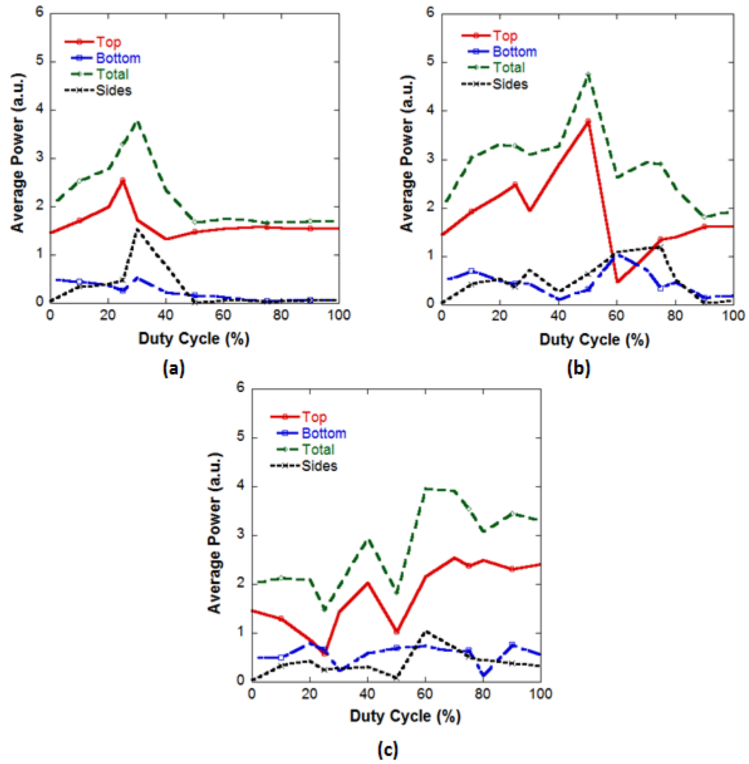

Figure 3: Output power for grating width: (a) 125nm, (b) 230nm, (c) 460nm for ITO layer thickness of 78nm

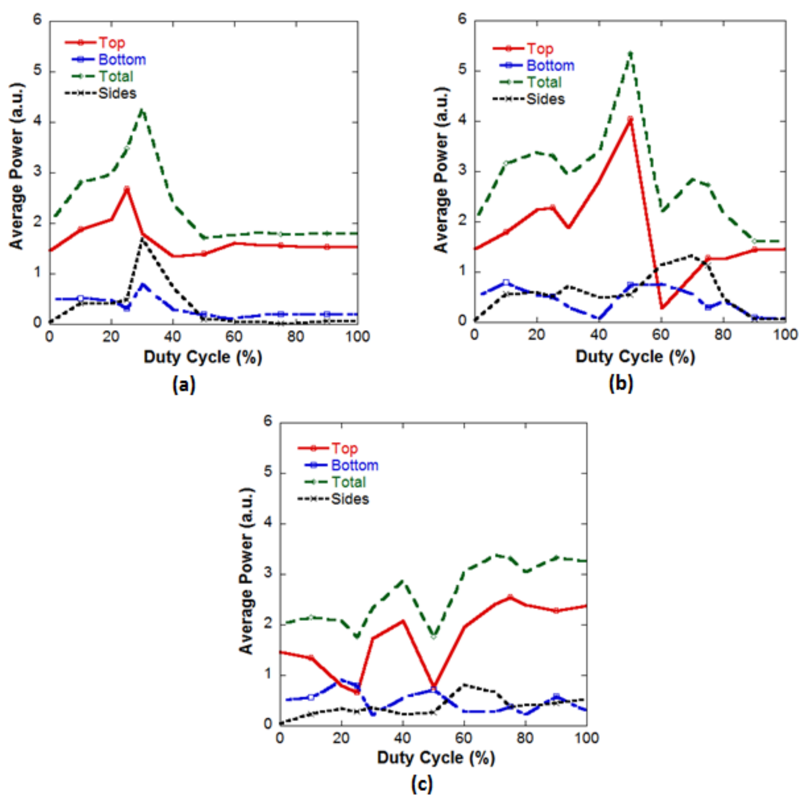

Figure 4: Output power for grating width: (a) 125nm, (b) 230nm, (c) 460nm for ITO layer thickness of 230nm

To better explain our above data, we study the electromagnetic (EM) field distribution in our LED. These results show that adding sapphire to the LED changes the standing wave conditions in the LED. Fig. 5(a) shows that the worst case thickness causes the light to strongly propagate through the n-GaN and sapphire substrate in the interference pattern. The best case thickness causes the standing waves in Fig. 5 (b) to have strong constructive interference at the ITO to air interface, while the EM waves in the n-GaN and sapphire layers destructively interfere and the EM field is almost completely negated.

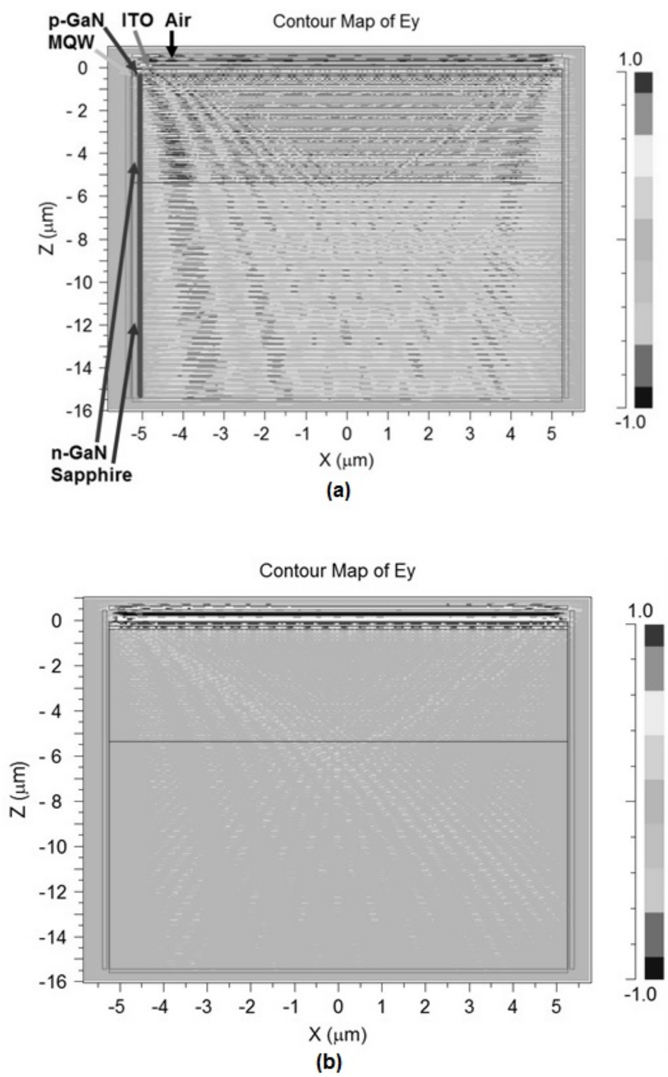

Figure 5: Electromagnetic fields in the LED under Sapphire with ITO 78nm (a)worst case = 10,032nm (b) best case = 10,050

Conclusion

This paper successfully shows that for sub-wavelength grating dimensions, by varying grating duty cycle, we can improve light extraction efficiency. With 230nm grating width and 50 % duty cycle, which is a full wavelength period and a half wavelength cell width, light extraction efficiency can be improved by 136.77% and 165.67% for 78nm and 230nm ITO layer thicknesses, respectively.

The next step would be to work on 3D GaN LED Nano-ITO grating simulations. Not only is this critical for accuracy of the model, especially when considering nano-structure gratings whose interactions depend on a three dimensional crystal structure, but also it allows one to create more complex grating structures. To the best of our knowledge, there are currently no publications detailing the simulation of three dimensional structures on GaN devices. Although the three dimensional model is more accurate and can simulate more features, the tradeoff is in the vast difference in computation requirements. The best way to approach the simulation is to study and improve the device model since it will not only reduce the hardware requirements but also will reduce the simulation time to speed up the research cycle.

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Appendices

• 1. Summary of Functional Requirements

Simulating LED CAD compare how the variables under test affect the light extraction efficiency. Graphing and analyzing the collected data finds the optimum condition where the top light monitor reads the highest light intensity and the bottom and side light monitors read the lowest light intensity. The total light intensity shows how much light exits the different LED CAD models.

• 2. Primary Constraints

Only two variables under test can be studied because of simulation time for each LED CAD model. More data points are taken around the maximum to show the true optimum condition. Building and simulating various LED CAD models accurately is time consuming and computer power intensive.

• 3. Economic

Elemental gallium is not found in nature, but it is easily obtained by smelting. It is obtained as a by-product of mining and processing other metals, notably aluminum, zinc and copper, and is produced by any nation that produces these metals. Once gallium is obtained, semiconductor companies, like Soitec and Sumitomo Electric Industries, use Smart Cut technology to manufacture engineered GaN substrates for LED lighting applications. Other technologies are used such as hydride vapor-phase epitaxy (HVPE) for the deposition of GaN layers on sapphire substrates. Costs accrue from the beginning stages of processing metals to acquire pure gallium to the later stages of slicing GaN wafers ready for LED lighting applications. Building LED CAD models and running simulations costs the price of the software and computer power. Analyzing this data will make the use of GaN wafers more efficient and increase life expectancy.

• 4. If manufactured on a commercial basis:

I estimate that about 100 billion units of gallium nitride LEDs will be sold per year. Manufacturing coast for each LED is about $500 dollars. Estimated price for each device depends on the commercial product. Profits per year and cost for the user to operate the device also depend on the commercial product being made.

• 5. Environmental

GaN LEDs having a longer lifetime will lower the waste compared to commercial lighting in the market now. This will improve different species environments and lifestyles. Also lighting for humans will be more convenient and nicer to the eye. Having dimmers and a nice white light will better the environment. Smart lighting will also add to convenience and efficiency.

• 6. Manufacturability

The cost of manufacturing GaN wafers can be significantly high but new technology is currently emerging and lowering these costs. Increase in demand will improve design approaches.

• 7. Sustainability

Temperature of the completed device may cause some issues. Thermal stress can degrade the light output over time. Different grating structures can improve the light extraction efficiency and thermal stress problems, which ultimately increases lifetime of the device.

• 8. Ethical

Utilitarian ethics will arise when designing the GaN LED. Decisions will be made to bring the highest good for everyone involved in the product, however the customer is the top priority. Decisions should be made consistent with the safety, health, and welfare of the public and factors that might endanger the public or the environment should be disclosed promptly. Bright LEDs should not be looked at directly and manufactures should state this fact. The technology used and its potential consequences should be understood by manufactures. Fabricating GaN wafers can involve hazardous chemicals and waste and this waste should be disposed of properly and safely. Excessive actions should be made to find and correct errors, no matter the costs.

• 9. Health and Safety

Bulk GaN is not toxic and biocompatible, which makes it perfect to use for implants in living organisms. However, GaN dust is an irritant to skin and eyes, which can be a health hazard. The light extraction efficiency of the LEDs may be so high it could damage eyes.

• 10. Social and Political

Improving LEDs efficiency and length of life impacts directly or indirectly a great deal of people. Direct stakeholders include electric and lighting companies. Having longer lasting lighting will make lighting companies sell less products because their products are lasting longer than before. They could also charge more for these products due to more expensive manufacturing costs and more extensive research. Electric companies would also feel an impact due to less power consumption by the more efficient LED lighting. Indirect stakeholders include anybody who helps the development of the LEDs. This includes UPS transporting and delivering parts to the manufactures. This would benefit UPS and create more business and profit. Less power would need to be generated by utility companies due to more efficient LEDs and smart lighting.

• 11. Development

I've learned new techniques in RSoft Fullwave in building LED models more efficiently. Also KGraph has been a very helpful tool in analyzing data fast and efficiently. It will be nice to use these graphs in showing my results to others.

Specifications and requirements

Table 2: Simulation of Nanoscale ITO Top Grating of GaN LED Requirements and Specifications

Marketing Requirements	Engineering Specifications	Justification
3, 4	Use RSoft Fullwave to simulate and calculate light extraction efficiency monitored at the top, bottom, and sides of the 2D LED structure.	RSoft Fullwave is used by colleagues and is trusted simulation software. Results from 2D CAD model simulations can give insight on how a 3D model will perform.
2,3,4	Simulate conical grating duty cycles from 10% to 100% at 10% increments.	To find the optimum grating duty cycle, data is taken exhaustively to find the true peak light intensity.
3,4	Keep light monitors consistent in all simulations (0.1um from the top, bottom, and sides of LED structure)	In order to compare light intensity data accurately, the monitors need to be arranged in a consistent manner no matter what variables are changing.
1,2,4	A sum of the light intensities (top + bottom + sides) will be calculated and graphed.	To compare how much light is emitted from the MQW region in the different models.
1,3,4,5	Simulate a no grating case for both ITO thicknesses.	To compare conical grating LEDs to conventional non-grating LEDs.

Marketing Requirements

1. Improves light extraction efficiency compared to a conventional LED.
2. Utilizes optimum ITO thickness, grating duty cycle, and grating dimensions.
3. Simulations use FDTD method to obtain accurate light extraction data from CAD models.
4. Deepen understanding of the filling factor’s effect on sub-wavelength gratings on GaN LEDs.
5. Draw some meaningful conclusions from the results.

Table 2 shows the requirements and specifications of simulation of nanoscale ITO Top Grating of GaN LEDs.

Parts List and Costs:

Table 3: Project Cost Estimation

Project Component	Estimated Costs	Actual Costs
RSoft Fullwave Software	$40k	$0 (Donation)
Labor	0	0