1. Introduction

Device simulations play an important role in device research. The equations that govern device physics are complicated and not easy to solve except for very simple devices using crude approximations. As devices become more complex, device researchers and designers turn to simulation tools that provide insight in the design and operation of devices. The job of the simulation tool developer is to research and devise models that will simulate various devices, develop the algorithms and computer code to solve the models, and present the results in an intuitive and useful way.

The motivation for this work was the desire to simulate various optoelectronic devices - electronic semiconductor devices that interact with light. The primary optoelectronic device of interest is the vertical cavity surface emitting laser, or VCSEL [1,2]. This semiconductor laser uses two reflectors, known as distributed Bragg reflectors or DBRs, that serve to reflect light back and forth across an active region. The active region amplifies the light until coherent emission occurs. Figure 1 shows a simplified diagram of a VCSEL structure. The focus of this thesis is on the models necessary to simulate optoelectronic devices. Results from specific examples, including a VCSEL, will demonstrate the use of these models.

There are three main problems with simulating the structure in Figure 1. First, VCSELs can use more than 150 layers of various materials. This complicates the simulations by requiring models that handle the material boundaries. Second, VCSELs use the many layers to obtain specific optical properties. These optical properties depend on the results of the electrical equations. Third, many unfavorable properties of VCSELs result from their thermal characteristics. The thermal models also couple to the electrical and optical simulations. To handle these problems, a device simulator must incorporate a set of specific features. Table 1 lists the key features for each of the main problem areas as well as some general features desirable in any simulation tool.

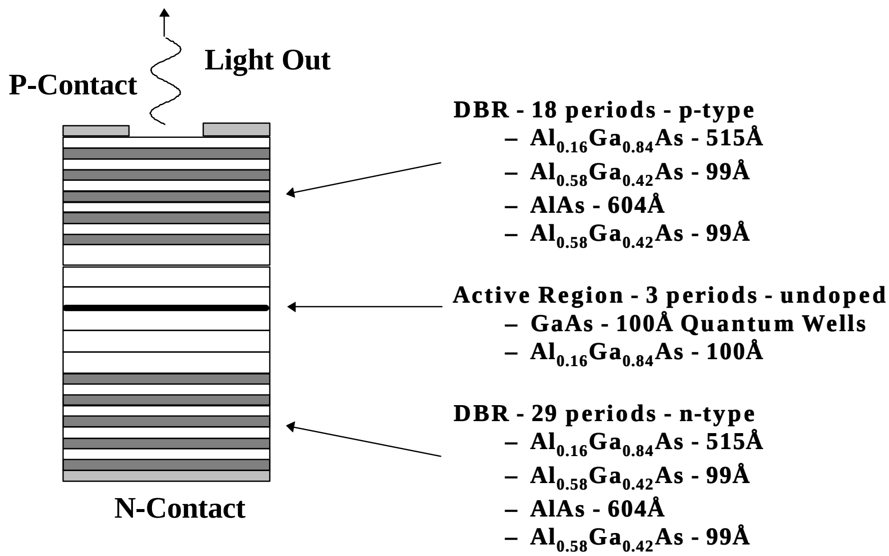

Figure 1 - Sample VCSEL structure

There are a number of simulators [3-10] that can address some of the features listed in Table 1, but none of them can address them all. PC-1D [3] can handle solar cells and photodetectors, but it limits the number of material layers that it simulates. HFIELDS [4] is more powerful in both the electrical and optical equations than PC-1D, but it can not simulate internal light generation or heat flow. FELES [5] uses an integrated electrical, optical, and thermal simulation, but it simulates edge emitting lasers as opposed to surface emitting lasers. MINILASE [6,7] is similar to FELES, but implements a more advanced quantum well model. Although, it also only simulates edge emitting lasers. TRENDY [8], FIELDAY [9], and ATLAS [10] are all more appropriate for commercial transistor applications. All incorporate advanced electrical and thermal models, but lack the optical equations that surface emitting lasers require. Reference [11] presents the most complete numerical model for VCSELs to date where the optical equations are very complete, but it too lacks some important carrier and energy physics.

Table 1 - Required features for simulating VCSELs

Problem Area	Feature
Electrical	General materials
	Large number of grid points
	High doping
	Incomplete ionization
	Thermionic emission
	Tunneling
	Quantum wells
Optical	Interface reflections
	Wavelength search
	Stimulated emission
Thermal	Boundary heat flow
	Lateral heat flow
	Temperature dependent parameters
General	Easy to use
	General purpose

As part of this research, the author developed the optoelectronic device simulation tool, SimWindows [12], in an attempt to solve the simulation problems associated with VCSELs. Its core is a one dimensional drift-diffusion simulator that adds all of the features in Table 1. Due to the one dimensional nature, SimWindows can not model all major aspects of VCSELs. However, this is the first attempt to model VCSELs from a pure physical point of view that requires only material parameters as input.

The simulator contains three basic solvers: a solver for each the electrical equations, the optical equations, and the thermal equations. These solvers pass information to each other, and when all three reach a solution simultaneously, the simulation is complete. Device simulations do not necessarily require all of the solvers. SimWindows always invokes the electrical solver, but it invokes the optical and thermal solvers depending on the nature of the device and the options that the user selects. VCSEL simulations require all three solvers.

The design of SimWindows is not just to model VCSELs because SimWindows implements all of the features listed in Table 1 in a general manner. The user can select features that are of interest and disable features that are unimportant. SimWindows also provides a large degree of flexibility. The user can easily add new material models or modify the existing material models. The purpose of creating a general easy to use tool was to give others an opportunity to experiment with SimWindows and provide feedback during its development. This feedback was invaluable. Although the concept of creating a general purpose simulator expanded the complexity and size of the computer code by at least a third, the benefits have been worth the extra time and effort.

SimWindows is currently available on the World Wide Web. Its present home page is at http://ucsu.colorado.edu/~winston/simwin.html. That location is likely to change in the future. Table 2 lists some facts about SimWindows. Figure 2 presents a screen shot of SimWindows 32 while simulating an AlGaAs/GaAs pn diode.

Table 2 - Facts about SimWindows version 1.4.2

Available Versions	16 and 32 bit
Operating System	Windows 3.1, 95, NT
Language	C++
Numeric Classes	63
Interface Classes	32
Total Lines	29,831
Compiler	Borland C++ v. 4.52
Win32s	required under Windows 3.1

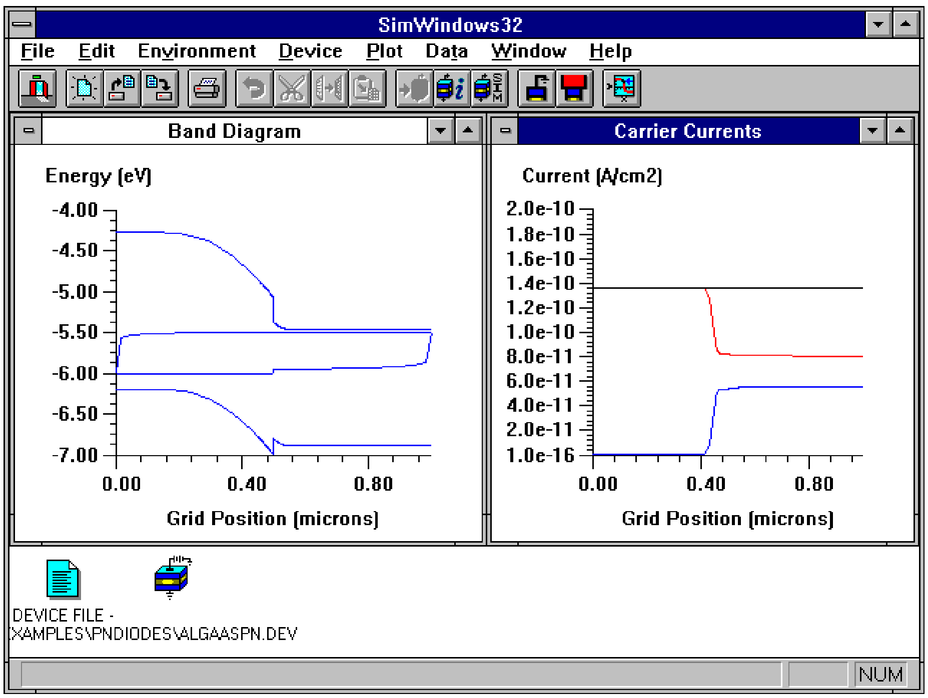

Figure 2 - Screen shot of SimWindows showing the results of a AlGaAs pn diode

This thesis consists of two parts. The first part includes this introductory chapter as well as the following three chapters. Chapter 2 will describe the complete mathematical model that SimWindows solves. It will explain how the model implements the various features listed in Table 1. Chapter 3 will demonstrate the use of the model on various practical devices. These include a complete VCSEL and a multi-quantum well solar cell. Chapter 4 will summarize these main chapters and propose some directions for future work.

The second part of the thesis includes eight appendices of supplemental information. Appendix A shows some tests that compare SimWindows results to analytical calculations. Appendix B lists the actual device files that SimWindows used to generate the results in this thesis. Appendix C is the User's Manual for SimWindows version 1.4.2. Appendix D is a complete list of symbols and definitions. Appendix E lists all of the of the continuous equations in the SimWindows model with their corresponding discrete equations appearing in Appendix F. Appendix G presents the derivations for specific equations, and Appendix H outlines various important mathematical functions.