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1998

Quantum Transport Simulations of Novel Compound Semiconductor Devices

by

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Dissertation

Presented to the Faculty of the Graduate School of

The University of Texas at Austin

in Partial Fulfillment

of the Requirements

for the Degree of

Doctor of Philosophy

The University of Texas at Austin
May, 1998

Quantum Transport Simulations of Novel Compound Semiconductor Devices

Approved by
Dissertation Committee:

Supervisor

Acknowledgements

I would like to acknowledge the help and support of all Team Neikirk members, especially Kiran Gullapalli. I must also thank the MBE group for growing wafers as well as their help in fabrication. I thank Dr. Maziar for her advice and tutelage on simulation matters, and Dr. Neikirk for his patience. Lastly, I thank my wife without whose help this dissertation would have been longer.

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Publication No._____________

Olin Lee Hartin, Ph.D.

The University of Texas at Austin, 1998

Supervisor: Dean P. Neikirk

As devices in the semiconductor industry tend to shrink below 0.1 μm quantum devices that work because of their small size, rather than in spite of it, become more attractive. It may be useful to simulate the operation of these devices whose behavior depends upon quantum tunneling and interference effects using comprehensive simulation tools.

In this work a two dimensional Schrodinger Poisson self-consistent simulator is described and demonstrated. Multi-valley coupling of effective mass equations is demonstrated and evaluated. A one dimensional Schrodinger Poisson self-consistent algorithm based on the tight binding formalism is also described and applied to heterostructure devices. Data from simulations based on these methods are compared with experimental data..

The methods developed allow the study of devices exhibiting quantum coherence effects combined with space charge effects in the presence of complex band structures and high electric fields. Such characteristics are present in a

variety of heterobarrier problems and in structures with ultra-thin oxides. Our self-consistent tight binding algorithm has been tested on several device structures.

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Chapter 1 Introduction

There are a number of novel devices that depend upon quantum tunneling and interference effects. Since some of these device ideas are difficult to test in the laboratory, the need to do optimization and inverse modeling in design of these devices suggests development of more comprehensive simulation tools.

Effective mass approximation-based Schrödinger Poisson simulation tools make it possible to rapidly simulate large device models. Convergence is an issue in part because the density of states function is highly nonlinear in these problems. The tight binding Hamiltonian can be used to do simulations of a range of materials including band mixing between materials. Valley mixing affects carrier concentration and transmission in devices with complex structures. Less rigorous methods based on effective mass approximations may be used to approximate these effects. However, there are differences between simulations based on coupling of effective mass equations and on the tight binding approximation.

One class of novel devices is simulated with these methods. The quantum storage device (QSD) is one of the new class of novel devices based on simulations and laboratory measurements. The addition of simulation methods introduced here add to the understanding of this device. Self-consistent solutions to the Schrödinger and Poisson equations have been widely used to identify both qualitative, and with varying degrees of success, quantitative behavior of Double Barrier Resonant Tunneling Diodes (DBRTDs).[1,2]. Self-consistent solutions are essential because quantum well diodes often incorporate lightly doped layers, and the resulting space-charge effects can significantly influence device characteristics[3,4].