

# Preface

Part of my lecturing work in the School of Mathematics at the University of Leeds involved teaching quantum mechanics and statistical mechanics to mathematics undergraduates, and also mathematical methods to undergraduate students in the School of Electronic and Electrical Engineering at the University. The subject of this book has arisen as a result of research collaboration on device modelling with members of the School of Electronic and Electrical Engineering.

I wanted to write a book which would be of practical help to those wishing to learn more about the mathematical and numerical methods involved in heterojunction device modelling. I have introduced only a comparatively small number of topics, and the reader may think that other important topics should have been included. But of the topics which I have introduced, I hope that I have given the reader some practical advice concerning the implementation of the methods which are discussed. This practical advice includes demonstrating how the implementation of the methods may be tailored to the specific device being modelled, and also includes some sections of computer code to illustrate this implementation. I have also included some background theory regarding the origins of the routines.

I have sought to produce an appropriate blend of theory and practical tips. I have not sought to obtain complete solutions—for example,  $I$ – $V$  characteristic results have not been included. The mathematical treatment may not be rigorous enough for the likes of the hardened mathematician, and the device treatment may not be detailed enough for the hardened device modeller. But I hope that I have given a balanced blend of both aspects, so that the reader will be confident enough to tackle subjects which are not covered in this book, particularly in relation to heterojunction device modelling.

When applying the mathematical and numerical routines, I have concentrated mainly on the heterojunction devices MESFET and the HEMT. In particular, the modelling of the HEMT involves problems which are encountered in many situations—coupled highly nonlinear sets of equations, and the explicit solution of the Schrödinger equation. An understanding of the methods involved in the modelling of these devices should give the reader confidence to apply them to other devices. The discretisation of the modelling equations will be described mainly in terms of finite differences.

Part I of the book introduces the basic physical theory which forms the backbone of semiconductor device modelling. The subjects of quantum mechanics and statistical mechanics are introduced in detail, and targeted towards device applications. This Part also includes discussions of the Effective Mass Approximation, the density of states in the quantum wells which form in HEMTs, the Boltzmann Transport Equation from which the transport equations are derived, and the Wigner Transport Equation.

In my collaborative work on device modelling, I have used all of the methods described in Part II to obtain results in device simulations. Part II presents the discussion of some of the main mathematical and numerical methods which are to be applied to the solution of the coupled modelling equations. Chapters include introductions to the Newton method in its specific application to device modelling, upwinding, a phaseplane method which can be used to obtain solutions of the device equation in a way that enables these equations to be easily modified when the device model changes, the multigrid method, a chapter on the numerical solution of the Schrödinger equation, and a chapter on rectangular grid generation. I have also included a chapter on Genetic Algorithms, although this is considered by some to be a method more closely associated with “softer” disciplines. This method cannot be used solely for a full device simulation, but I have found the method to be very useful in solving some subsidiary optimisation problems. Part II also contains short sections of code, written in simple C++, to illustrate how some of the methods can be implemented.

I have written this book for anyone who is interested in learning about, or refreshing their knowledge of, some of the basic mathematical and computational aspects of device modelling. This could include upper-level undergraduates, both mathematicians who would like to enter the world of device modelling, and electronic engineering students who would like an introduction to some of the mathematical and numerical methods applied to device modelling. Also included would be those wishing to learn about, or refresh their knowledge of, the basic subjects of quantum mechanics and statistical mechanics. The work could also be of interest to researchers already working on device modelling, and who would perhaps like to get a different perspective on the subject. I have included a section on simple coding in C++; this should be of use to programmers using other languages, and to undergraduates who have not had much exposure to programming at all.

There is a website associated with this book. It contains a list of errata, together with complete working listings of some of the programmes described in the book. Visit the Springer website at [www.springer.com](http://www.springer.com).

Finally, I would like to acknowledge the influence of two people. To Chris Snowden who, as Professor of Microwave Engineering at the University of Leeds, communicated his endless enthusiasm to all who came into contact with him. Also to Peter Landsberg who, as my research supervisor many years ago at Cardiff, taught me that I should not always trust the equation

$$A = B + \text{wishful thinking.}$$

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