Preface

Within this volume, we have attempted to present a comprehensive picture of the state of the art in transport modeling relevant for the simulation of nanoscale semiconductor devices. At the time of the publication of this book, advances in conventional planar semiconductor device scaling have resulted in production devices with gate lengths approaching 22 nanometers (at the time of writing this preface), while research devices with gate lengths of just a few nanometers have been demonstrated. The semiconductor industry has been dominated by Si based Metal Oxide Semiconductor (MOS) transistors for over 40 years. However, at present, there is an increasing drive to integrate a diversity of materials such as III–V compound channel materials and high insulator dielectrics, and the introduction of radically new materials such as graphene. At the same time, there have been extraordinary advances in new types of self-assembled materials such as carbon nanotubes, and semiconductor nanowires, which offer the potential for new families of fully three-dimensional devices that will allow scaling to continue to atomic dimensions. As characteristic length scales decrease, the physics of transport changes dramatically. For large dimensions compared to the mean free path for scattering (and the related phase coherence length), the semi-classical diffusive picture of charge transport holds, governed by the Boltzmann transport equation (BTE). On the other hand, for very short length scales, much less than the scattering mean free path, transport is coherent, and described in a purely quantum mechanical framework in terms of current associated with probability flux, usually from some idealized reservoir of carriers, i.e. contacts. The actual situation in current nanoscale devices is somewhere in between these two pictures, which in the past has been referred to as a *mesoscopic* system (somewhere between microscopic and macroscopic). This regime perhaps the most interesting in terms of phenomena, but the most difficult to theoretically describe, in which both quantum mechanical phase coherent phenomena co-exist with phase randomizing, dissipative scattering processes, which requires a general theoretical approach capable of dealing with both on an equal footing. In this book, we compile different approaches to the problem of transport in mesoscopic semiconductor systems, ranging from semi-classical to fully quantum mechanical, in order to understand the advantages and limitations of each, as well as elucidating the complex and interesting phenomena encountered in ultra-small devices.

In Chap. 1, we begin with an introduction to semi-classical device modeling, starting from the BTE, and deriving the associated moment equations leading to the widely used drift-diffusion and energy transport models, with different approaches for extraction of the transport parameters, and applications of this approach in some new novel energy conversion and sensing technologies. Chapter 2 considers the inclusion of quantum mechanical effects such as tunneling and quantum confinement within the popular ensemble Monte Carlo (EMC) method for the solution of the semi-classical BTE, as well as the treatment of many body interactions between particles as well as between particles and impurities within a molecular dynamics framework. Chapter 3 introduces the full-band EMC method, in which the complete electronic bandstructure is used in the description of the electron and hole dynamics as well as scattering processes semi-classically. A formalism based on the Pauli Master Equation is then introduced which allows for simulation of quantum transport within a similar framework to the BTE, and which is applied to some specific nanoscale structures where quantum effects are important such as resonant tunneling diodes (RTDs). Chapter 4 provides the general theoretical framework for quantum transport starting with the Liouiville-von Neumann equation, and then the various approximation schemes which lead to various forms of Master equations, including the Pauli and Boltzmann formalisms. Chapter 5 gives an overview of quantum transport based on the Wigner Function method, which utilizes a quantum mechanical distribution function in place of the semi-classical distribution function appearing in the BTE to obtain the Wigner–Boltzmann equation. Numerical approaches for the solution of the Wigner–Boltzmann equation are discussed, and the application to quantum devices such as RTDs and nanoscale transistors presented. Chapter 6 provides a description of quantum transport from a scattering matrix, wavefunction approach, based on the so-called Usuki method. Applications to transport through various prototype nanostructures such as quantum dots, nanowires and molecular systems are presented, including spin dependent phenomena which can be described within the same framework. The inclusion of scattering in real space within the Usuki method is then described, and its application to nanoscale MOSFETs presented. Chapter 7 details an atomistic approach to transport appropriate for nanoscale systems, based on the empirical tight binding method for large systems of atoms such as quantum dots and nanoscale transistors.

We deeply acknowledge the valuable contributions that each of the authors made in writing these excellent chapters that this book consists of.

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