Physical Models of Semiconductor Quantum Devices

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Preface

The history of technology development is epitomized in Moore's law. Industrial deep-submicron and laboratorial nanometer process technologies have already been fabricating electronic and optical components containing only a few active electrons, and the geometrical sizes of these components are comparable with the characteristic wavelength of the electrons. However, the advanced multimedia infrastructure and service in the future demand further developments in the chip's capability.

Photonic integrated circuits (PICs) are currently orders of magnitude larger in physical dimensions than their microelectronic counterparts. Field-effect-type transistors have reached lengths on the order of 50 nm, while in contrast, passive optical devices, also those based on photonic crystals, have sizes on the order of one photon wavelength. The sizes of active devices are even larger, essentially depending on the matrix element of the interaction. In order to pursue the steady increase in integration density in photonics such that it rivals the microelectronic footprint size, nanostructure-based high index of refraction and metallic behavior (negative epsilon) are two mostly studied fundamental issues to shrink optical component sizes and to tackle the sub-wavelength limit.

Nanotechnology has been named as one of the most important areas of forthcoming technology because they promise to form the basis of future generations of electronic and optoelectronic devices. From the point view of technical physics, all these developments greatly reduce the geometric sizes of devices, and thus the number of active electrons in the system. Quantum mechanical considerations about electronic states, electron transports and various scattering processes including light-matter interaction, are thus crucial. However, the theoretical study is extremely difficult. My first numerical simulation work about a three-dimensional energy band structure calculation in 1995 took more than 6 months to complete for one bias-configuration of a nanoscale metal-oxide-semiconductor field-effect transistor (MOSFET). With today's computation workstations the CPU time is reduced to be less than 24 hours.

In general, today's experimental and theoretical works are very much separated. The laboratory works are still largely based on try-and-error, while the theoretical models are over simplified as compared with the complexity of real devices. Ideally to be cost effective, experimental and theoretical works are to be coordinated in such a complementary way that we try to analyze and understand the experimental results, then use the understanding to guide further experimental works, which in their turn serve as the feedback to modify and improve the theoretical model. By this, we expect an optimized device and a valid as well as effective theoretical device model.

The main purpose of the book is to discuss electrons and photons in and through nanostructures by the first-principles quantum mechanical theories and fundamental concepts (a unified coverage of nanostructured electronic and optical components) behind nano-electronics and optoelectronics, the material basis, physical phenomena, device physics, as well as designs and applications. The combination of viewpoints presented within the book can help to foster further research and cross-disciplinary interaction needed to surmount the barriers facing future generations of technology design.

Many specific technologies are presented, including quantum electronic devices, resonant tunneling devices, single electron devices, heterostructure bipolar transistors (HBTs) and high electron mobility transistors (HEMTs), detectors, and infrared sensors, lasers, optical modulators. It contains essential and detailed information about the state-of-the-art theories, methodologies, the way of working and real case studies, helping students and researchers to appreciate the current status and future potential of nanotechnology as applied to the electronics and optoelectronics industry.

In nanophotonics we will concentrate on local electromagnetic interactions between nanometric objects and optical fields (non-linear optics in nano- and microstructured photonic crystals) at the level of systems of nanostructures, into larger density on interfaces, which in turn leads to intriguing collective effects, such as plasmonics or multiple reflection and refraction phenomena.

The major task here is that the system at working condition is no longer static. Rather, it can only properly be described by including dynamic Maxwell and time-dependent Schrödinger equations. Furthermore, because the numbers of atoms and electrons in the real devices are huge, while the quantum mechanical Monte Carlo simulation requires too much computer memory and computer time, we will introduce top-down and bottom-up numerical ways that fundamentally we emphasize the quantum mechanical Monte Carlo simulation, while at the same time, we apply the large-system (cluster) tight-binding numerical method to study the device performance property (where the input parameters in the tight-binding method come from the study of bridging nano to micro scales).

Finally we will examine the processing—structure relationship. The state of nanostructures during the period that one monolayer exists—before being buried in the next layer—determines the ultimate structure of the nanostructure, and thus its properties. This part of the book takes into consideration the following potential influencing factors in solid-state growth techniques such as metalorganic vapour phase epitaxy (MOVPE): crystal defects, void structure, grain structure, interface structure in epitaxial films, reaction-induced structure, strain-induced self-formed quantum dot structures, through the use of MOVPE to produce quantum structured semiconductors.

This book provides a solid foundation for the understanding, design, and simulation of nano-electronic and optoelectronics devices. It will be of interest to researchers and specialists in the field of solid state technology, electronics and optoelectronics. It can also serve as a textbook for graduate students and new entrants in the exciting field. This book takes the reader from the introductory stage to the advanced level of the construction, principles of operation, and application of these devices, and puts readers immediately in a position to take their first steps in the field of computational nano-engineering and design. Results and conclusions of detailed nano-engineering studies are presented in an instructive style. Numerous references, illustrations, basic computation subroutines provide further support in this fast-emerging field. This book is designed as a self-contained introduction to both the understanding and solution of theoretical and practical design problems in nano devices.

Stockholm, Sweden Ying Fu
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