Numerical Analysis for Semiconductor Devices

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Notation

q	Electronic charge, 1.6×10^{-19}C.
$\varepsilon(=\varepsilon_s \varepsilon_0)$	Dielectric constant, $\varepsilon_0 = 8.86 \times 10^{-14}$ F/cm, $\varepsilon_s = 12$ for silicon.
m_e, m_h	Electron and hole effective masses.
h	Planck's constant, 6.63×10^{-34} J · s (chapter 2); division-point spacing (chapters 3–9).
k	Boltzmann's constant, 1.38×10^{-23} J/°K (chapter 2); time steplength (chapters 4–9).
$\mathscr{E}, \mathscr{E}_G$	Energy, bandgap energy.
T	Temperature.
θ	Boltzmann factor $[q/(kT)]$.
n_i	Intrinsic free-electron density.
n, p	Electron and hole densities.
N_d, N_a	Donor and acceptor concentrations.
Γ	Effective doping concentration $(N_d - N_a)$
ψ	Potential.
ϕ_n, ϕ_p	Electron and hold quasi-Fermi potentials.
$\mathbf{E}, E$	Electric field in vector and scalar, $\mathbf{E} = -\text{grad}\ \psi$.
μ_n, μ_p	Electron and hole mobilities.
D_n, D_p	Electron and hole diffusion constants.
$\mathbf{J}_n, \mathbf{J}_p, J_n, J_p$	Electron and hole current densities in vector and scalar.
t	Time.
G, U	Generation and recombination rates.
α_n, α_p	Electron and hole ionization rates.
τ_n, τ_p	Electron and hole lifetimes.

Preface

More than thirty years have elapsed since the advent of the semiconductor device. Shockley established a rigid theoretical basis for device analysis in his 1949 paper, where the basic equations are presented in exactly the form that is now used.

Thereafter, a tremendous number of technical papers appeared that followed this basis and dealt with the analysis of the different devices in various operation modes. For the first fifteen years, the analysis was implemented largely in such a manner that closed-form solutions were deduced from the basic equations under some simplifying assumptions.

Meanwhile, however, such methodology was recognized to have only limited applicability, especially when a unified device model was desired. This understanding led to the introduction of numerical analysis under the name of *device modeling*, which has evolved markedly in the past fifteen years, simultaneously supported by the enormous progress in computer performance.

As a result, contemporary device modeling has attained, at least among specialists, such a high level that even two-dimensional transistor analysis for DC steady state, as well as time-dependent problems, is implemented on high-performance computers that yield solutions within a reasonable time limit.

In view of this situation, numerical analysis is expected to become so popular that a large number of researchers and engineers will be concerned largely with it, although not necessarily as specialists. In fact, as computer performance steadily increases, problems that are moderately difficult today, such as exact one-dimensional modeling, will in the near future be studied and practiced commonly by many people, including students specializing in electronics.

With the aforementioned background, this book was written for numerical analysis of bipolar devices in general, with the intention of characterizing it in several ways. First, a detailed description is given in each relevant chapter for the derivation of discrete-form equations from the original differential equations, so that readers can easily write computation programs based on their own understanding. This distinguishes the book from many papers on device modeling presented in technical journals, where the detailed formulation is not always given, either because of space limitations or for other reasons.

Second, the numerical methods are designed in such a way that they are commonly applicable without an essential change in computer algorithm to many different types of devices, such as diodes, transistors, and thyristors, as well as many operation modes, such as DC steady state and nonsteady transient. This is especially true for chapters 4–6, devoted to one-dimensional models, whose validity has been proved through many practices in device design and characterization. A common concept in these one-dimensional models is extended to the two-dimensional analysis of chapter 7, based on the Newton-SLOR method, where a one-dimensional line segment is treated as a unit block.

Fourth, engineering aspects of modeling were considered by providing each relevant chapter with a number of realistic computation results, through which readers will understand the meaning and applicability of numerical analysis as a useful tool for device design.

Finally, two supplementary chapters, 8 and 9, were added. In chapter 8, a special case of two-dimensional analysis is discussed for reverse-biased *p-n* diodes concerning an estimate for breakdown voltages, where Poisson's equation is solved by employing the finite-element method as the only exception. Chapter 9 is devoted to the hybrid two-dimensional model, which will find various applications in many realistic problems because it characteristically includes two-dimensional effects without requiring as much computation time as the exact two-dimensional analysis.

I hope that this book will be used by many people willing to study the implementation of numerical device analysis, as well as by those willing to practice it in research and development and in device design. I hope, also, that knowledge of numerical analysis contributes to predicting characteristics of some of the devices that will appear in the future.

Contents

List of Figures

List of Tables

1 General Concept

Definition of Device Modeling

Device modeling is the technique for developing a model by means of which the actual behavior of a device can be simulated theoretically. Consider, for instance, a transistor, as illustrated in figure 1–1. Fabrication of the transistor involves many steps, which follow a number of prescribed design conditions—for example, resistivities for a starting material and an epitaxial layer, junction depths and surface resistivities for a number of impurity-diffusion processes, and lateral sizes for emitter and base areas. These quantities are called *device-design parameters*. A reasonable transistor model will be able to predict the electrical characteristics exhibited by the finished samples. These will include static current versus voltage characteristics, current-amplification factors, and cutoff frequencies or switching characteristics.

In general, actual device characteristics are functions of the design parameters. Therefore, the model must generate accurate theoretical results for an arbitrary set of design-parameter values.

The concept of modeling has only recently become a topic considered by device researchers and design engineers. However, the modeling concept itself originates in Shockley's paper published in 1949, which established the theoretical foundation for the junction diode and the transistor.[1] Starting from a set of differential equations, Shockley demonstrated a very clear view of the behavior of the semiconductor device. He did so almost immediately after the invention of the transistor itself by his own group.

Such a theoretical treatment was called *device analysis*, rather than device modeling. However, the difference between these two concepts is inconsequential here. It is sufficient to understand that the performance of device analysis for the purpose of developing a model is called device modeling.

The basic differential equations for device modeling include those for the current transport of electrons and holes, both consisting of a diffusion-current and a drift-current component. The drift component is represented as the product of the carrier density and the electric field. Since both of these are unknown variables, the transport equations are nonlinear.

As will be discussed later, the nonlinearity involved is of an exponential type, which deviates strongly from a linear relation. This strong nonlinearity