THE PHYSICS OF SEMICONDUCTORS

WITH APPLICATIONS TO OPTPELECTRONIC DEVICES

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KEVIN F. BRENNAN

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with applications to optoelectronic devices

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CAMBRIDGE
UNIVERSITY PRESS

PUBLISHED BY THE PRESS SYNDICATE OF THE UNIVERSITY OF CAMBRIDGE
The Pitt Building, Trumpington Street, Cambridge, United Kingdom

CAMBRIDGE UNIVERSITY PRESS
The Edinburgh Building, Cambridge CB2 2RU, UK http://www.cup.cam.ac.uk
40 West 20th Street, New York, NY 10011-4211, USA http://www.cup.org
10 Stamford Road, Oakleigh, Melbourne 3166, Australia

First published 1999

Printed in the United States of America

Typeset in Sabon 10.25/13pt. and Antique Olive in LaTeX 2ε [TB]

A catalog record for this book is available from the British Library

Library of Congress Cataloging in Publication data

Brennan, Kevin F., 1956–

The physics of semiconductors : with applications to optoelectronic devices / Kevin F. Brennan.

p. cm.

Includes bibliographical references.

ISBN 0-521-59350-6

1. Semiconductors. 2. Optoelectronic devices. I. Title.
QC611.B75 1999
621.3815'2 – dc21 98-29503
CIP

ISBN 0 521 59350 6 hardback
ISBN 0 521 59662 9 paperback

THE PHYSICS OF SEMICONDUCTORS

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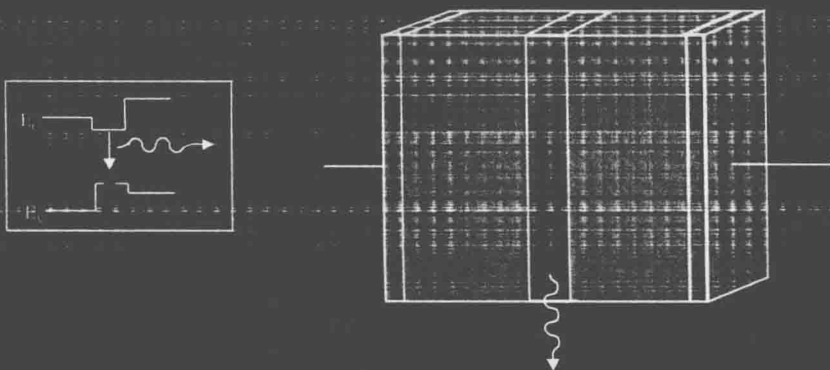

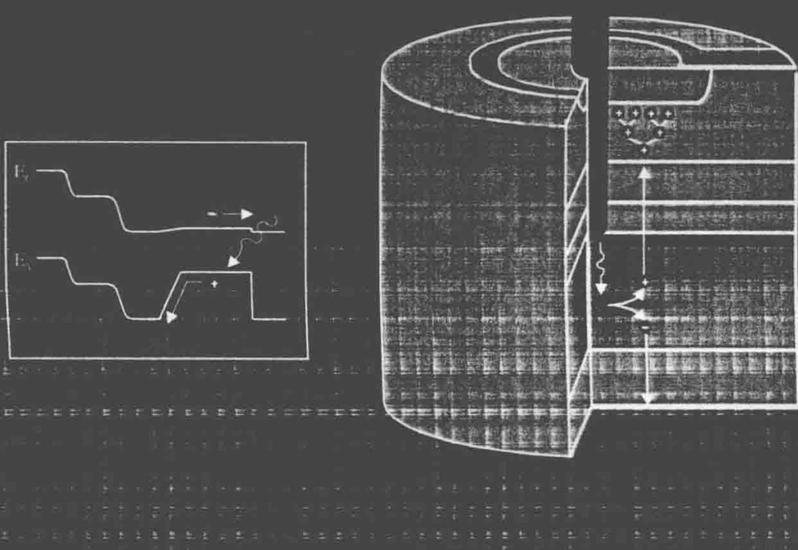

KEVIN F. BRENNAN

The Physics of Semiconductors

Modern fabrication techniques have made it possible to produce semiconductor devices whose dimensions are so small that quantum-mechanical effects dominate their behavior. This book describes the key elements of quantum mechanics, statistical mechanics, and solid-state physics that are necessary in understanding these modern semiconductor devices. Theoretical results are illustrated with reference to real devices such as photodiodes, flat-panel displays, and metal-oxide–semiconductor field-effect transistors.

The author begins with a review of elementary quantum mechanics and then describes more advanced topics, such as multiple quantum wells. He then discusses equilibrium and nonequilibrium statistical mechanics. Following this introduction, he provides a thorough treatment of solid-state physics, covering electron motion in periodic potentials, electron–phonon interactions, and recombination processes. The final four chapters are devoted exclusively to actual applications, ranging from simple junctions to the latest electroluminescent devices.

The book contains many homework exercises and is suitable as a textbook for electrical engineering, materials science, or physics students taking courses in solid-state device physics. It will also be a valuable reference for practicing engineers in optoelectronics and related areas.

Further material related to this book can be found on the worldwide web at: http://www.ece.gatech.edu/research/labs/comp_elec/

Kevin Brennan received his B.S. degree from the Massachusetts Institute of Technology and his M.S. and Ph.D. degrees from the University of Illinois, Urbana-Champaign. He is a Professor and Institute Fellow in the School of Electrical and Computer Engineering at the Georgia Institute of Technology. He was the recipient of a National Science Foundation Presidential Young Investigator Award and is the author of more than 110 technical articles. Professor Brennan has served as a consultant to various industrial and governmental organizations and holds several U.S. patents for his work on avalanche photodiodes.

To my mother and the memory of my father

Preface

The maturation of epitaxial crystal growth capabilities, such as molecular-beam epitaxy and chemical beam epitaxy, has enabled the realization of a host of new ultrasmall semiconductor devices. Aside from the feature size reduction of conventional semiconductor devices, particularly transistors, a totally new class of semiconductor devices has been invented. These structures, called superlattices/multiple-quantum-well devices, consist of alternating layers of different semiconductor materials, often measuring only a few atomic layers thick. These new semiconductor devices operate well within the range in which quantum-mechanical phenomena become prevalent. As a consequence, most new semiconductor devices behave according to quantum-mechanical effects rather than classical effects. Therefore the understanding of these new device types requires a firm grounding in the basics of quantum mechanics. It is the purpose of this book to introduce the engineering student, particularly those interested in studying solid-state devices, to the principles of quantum mechanics, statistical mechanics, and solid-state physics. Following this introduction, the physics of semiconductors and various device structures is examined.

The book contains fourteen chapters in total. The first four chapters are concerned with the standard principles of quantum mechanics for a one-particle system. I have attempted to condense the vast literature on this subject into just four chapters that will present the salient features of quantum mechanics. I have included a few topics, most notably a short presentation on relativistic quantum mechanics, for completeness. The instructor may elect to skip different sections as he or she sees fit. Sections in the Table of Contents marked by a † are optional, in the sense that material following that section does not directly depend on the material within that section. The first three chapters deal with problems that can be solved exactly in quantum mechanics. I feel that it makes the most sense to show first all the systems that can be solved exactly, including relativistic ones, before jumping to more complicated yet more interesting problems. Chapter 4 presents approximation methods, most notably perturbation theory, both time dependent and time independent. Armed with these principles, the student has most of the essential features of quantum mechanics needed to understand the workings of semiconductor devices.

Beginning with Chapter 5, the basic principles of statistical mechanics are presented. Equilibrium statistical mechanics is covered in Chapter 5, while nonequilibrium statistical mechanics is discussed in Chapter 6. In Chapter 6 the Boltzmann equation is derived and the basic modeling equations for semiconductor device simulation, the drift-diffusion and the Poisson equations, are developed. The chapter also includes a brief discussion of superconductivity.

Again, one may elect to include or omit this section. I would strongly urge the instructor to present this material since I have repeatedly found that the students' imagination is greatly sparked by this material. I personally believe that every solid-state engineer should have some understanding of the workings of superconductors. This is especially true after the recent discovery of high-temperature superconductors.

Chapter 7 begins the introduction to solids. Chapter 7 focuses on multielectron systems, molecular formation, energy-band formation through the tight binding approach, and crystalline symmetries. The behavior of electrons in a periodic potential is the subject of Chapter 8. Topics such as effective-mass theory, the Brillouin zone, the nearly-free-electron model, and cellular methods are included. Lattice vibrations and phonons are presented in Chapter 9. Chapter 10 concludes the presentation of the underlying physics of semiconductors by focusing on generation and recombination processes.

The balance of the book, Chapters 11–14, is devoted to device applications. Specifically, I discuss junctions in Chapter 11, detailing the workings of the most important junction types in both equilibrium and nonequilibrium. Photonic detectors and detection are the basis of Chapter 12. Photonic emitters are presented next in Chapter 13. The book concludes with a discussion of field-effect devices in Chapter 14. Obviously the choice of topics is not exhaustive. Many important topics have been omitted, particularly bipolar junction transistors, which are briefly discussed only in Chapter 12. My omission of many topics is due to the vastness of the subject matter. I have chosen to focus on junctions, detectors, emitters, and field-effect transistors since these are the most important devices in compound semiconductor device applications.

In writing such a book, I have obviously borrowed from those whom have gone before, and I am certainly indebted to many references. I have tried to include a full list of all the references that I have contacted at the end of the book.

From a pedagogic point of view, I have developed this book from notes I have written for a three-quarter first-year graduate-level course given in the School of Electrical Engineering at the Georgia Institute of Technology. Typically, I teach virtually all the material in Chapters 1–4 in the first quarter. In the second quarter, all of Chapters 5–8 and Section 9.1 of Chapter 9 are covered. The material in Chapters 10–14 is typically covered in a third-quarter class on semiconductor devices that follows the previous two quarters.

I would like to thank my many colleagues at Georgia Tech and elsewhere for their interest and helpful insight. I am particularly indebted to Dr. W. R. Callen, Jr., for his many suggestions throughout the writing of this book. I am also indebted to the many students at Georgia Tech who have taken the courses from which this book was developed. Their incisive criticisms, both during and after the courses, have been most helpful. In particular, I would like to thank Ali Adibi for his careful and critical reading of versions of the manuscript. I would also like to thank Joel Jackson for electronically coding all the figures, Enrico Bellotti for revising the computer codes and generating many figures, and William Darkwah for his work on translating the computer codes into C. I am also grateful to Maziar Farahmand for his help in some of the mathematical derivations in the text.

Finally, I would like to thank my friends and family for their enduring support.

Atlanta, January 1998

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†Section can be omitted without loss of continuity.

1

Basic Concepts in Quantum Mechanics

Quantum mechanics forms the basis of modern physics. In a sense it is the parent theory about which we construct our view of the physical world. Briefly, quantum mechanics is the theory by which we describe the behaviors of subatomic and atomic particles, such as electrons, of which the macroscopic world is made. Although it is not necessary to treat macroscopic objects by use of quantum mechanics, the laws of quantum mechanics and their implications are completely consistent with Newton's Laws of Motion, which we know are applicable to most macroscopic objects. As we will see below, Newton's Laws of Motion are a special subset of quantum mechanics; quantum mechanics reduces to Newton's Laws at macroscopic dimensions.

Before we begin our study of quantum mechanics, it is of interest to explain why quantum mechanics is of importance in the study of modern electrical engineering. Many new areas of electrical engineering are based on developments that can be understood only through the use of quantum mechanics. Among these are the broad areas of

1. semiconductors and solid-state electronic devices,
2. electro-optics and lasers,
3. superconductors.

It would be fair to say that in the study of each of the above areas some knowledge of quantum mechanics is essential. In this book, some basic concepts in quantum mechanics are presented that are necessary in the study of the above-mentioned disciplines.

1.1 Introduction

The concept most basic toward the understanding of quantum mechanics is the concept of measurement. In classical physics, the range in which Newton's Laws of Motion apply, the question of measurement rarely is of fundamental importance. We tacitly assume that a measurement of a physical observable, say length, can be made unequivocally. In other words, we assume that everyone will obtain the same measured value of the length of an object at all times. In fact, this seems so obvious that we rarely discuss it at all. However, in quantum mechanics, there is no guarantee that one will always measure the same value of a physical observable at all times. The physical observables commonly measured – microscopic particles, energy, momentum, angular momentum, etc. – can be altered by the mere action of the measurement itself. As a result, one cannot definitively state what value of a particular observable a quantum-mechanical particle will have until a measurement of that observable has been performed. In addition, the measured value may be very different from one measurement to the next.

Let us first consider a simple example of measurement that can help us understand this uncertainty. Let us define the two sides of a coin as the only two possible states of the coin. The coin will always be in its final state in one of only two possible states, heads up or tails up (heads or tails). If the coin is flipped we expect then that the coin will end up either heads or tails after the coin has come to rest. In a sense, we have measured the state of the coin by examining what side is up after it has been flipped. The experiment that we will perform then is something like this. We start with a two-sided coin, heads and tails. The coin is in some initial state, either heads up or tails up. The coin is flipped, and it comes to rest with either heads up or tails up. Of course, we do not know which side is up or down until we examine the coin. By looking at the coin, we measure the state of the coin and decide if it is heads or tails.

Let us consider a variation on the above experiment. As we will see in Chapter 4, an electron also has two possible states that it can be in. These states are related to the spin angular momentum of the electron. As we will see, the spin angular momentum of an electron can be oriented in one of two possible ways. For convenience we call these orientations up or down and the state of the electron either spin up or spin down. A similar experiment to the flipping coin can be performed with an electron. Consider the case in which an electron is created through a beta decay of a nucleus. If we know nothing about the nature of the decay, we would expect to find the emitted electron in either the spin-up or the spin-down state with equal probability, just as we expect to find a flipped coin in either the heads or the tails state. It is important to recognize the fact that we do not know what state the electron is in, though, until we measure it. This is identical to the case of the coin: we do not know whether the coin is heads or tails until we look at it.

What, though, is the state the electron is in before we measure it? Intuitively, we would argue that it must be either spin up or spin down and just assume that its state is well defined at all times and that when we measured it we simply observed what state it was in. Quantum mechanics tells us that this is not correct. The electron is much like the flipped coin. One could ask the question, what state is the coin in before it comes to rest? In other words, is the coin heads or tails while it is spinning in the air? Such a question is ridiculous to ask about the spinning coin because the coin is not in a definite state, heads or tails, until after it has come to rest. The coin is in a definite state only after we have measured what state it is in. Quantum mechanics tells us that to ask the same question about the electron state before measuring it is also meaningless. The electron is not in a definite state until we have measured it. What seems strange about this argument is that we have grown used to the idea in classical physics that the external world is independent of ourselves. To the classical mind, the presence or the absence of the experimenter has no consequence on the results of the experiment. Quantum mechanics tells us that this is not true. The mere action of measurement alters the state of the system, changing it from an indefinite state (coin spinning in the air, electron moving through space) into a definite state (coin comes to rest in either the heads or the tails configuration; electron measured as having either spin up or spin down).

Although the analogy between the spinning coin and an electron is somewhat attractive, there is an important difference between these two situations. One can argue that although the state of the coin is unknown while it is flipping in the air, its final state, either heads or tails, is predictable based on its initial condition and the force applied to set it spinning. Although such a calculation may prove difficult, it is, at least in principle, tractable. Therefore the uncertainty in the final state of the spinning coin is due only to ignorance and not to something fundamental. However, for the electron this is not the case. As we discuss below, knowledge of the electron's state is inherently uncertain until a measurement is made.

The thought experiment described above indicates that there is an inherent uncertainty in the behaviors of microscopic particles. Essentially, the results of our thought experiment indicate that the electron is in an indefinite state until a measurement is made on it and that as a consequence there is an inherent uncertainty in the state of the electron before measurement. Let us carefully discuss this point. This implies that not only does the experimenter not know the state of the electron before the measurement but the electron itself does not know. In other words, there is no way one can know in advance precisely in what state the electron will be found on measurement. As mentioned above, this is completely foreign to classical physics. It would be akin to stating that the orbit of the Earth is uncertain and not predictable.

What proof do we have that the uncertainty in the state of the electron is fundamental and is not just a consequence of our own ignorance of the state of the electron? After all, one could argue that the electron is in a well-defined state unknown to us until we measure it. The uncertainty in that case is due only to ignorance on the part of the observer, not to any fundamental uncertainty in the nature of the electron's state itself. This is the uncertainty we ascribe to the flipping coin, that is, in principle we can predict with certainty which state it will finally be in but it is extremely difficult to do that in practice. To understand what is meant by uncertainty as applied to a quantum-mechanical entity, let us more clearly define quantum-mechanical uncertainty. The well-known Heisenberg Uncertainty Principle of quantum mechanics states that certain sets of conjugate observables cannot be simultaneously known with infinite precision. The Uncertainty Principle is most frequently written in terms of the uncertainties in the real space position Δx and linear momentum Δp_x of the particle as

$$(\Delta x)(\Delta p_x) \geq \hbar/2.$$

The above equation implies that the product in the uncertainties of the two physical observables, position x and linear momentum p_x, must be always greater than or equal to Planck's constant divided by 2π, written as $\hbar$. Physically, this states that the two observables, position and linear momentum, cannot be simultaneously known with infinite precision. The Uncertainty Principle states that the uncertainty in the knowledge of the values of canonical observables is fundamental.

We still have not clearly made an argument that would indicate that the uncertainty is fundamental. One could argue that there are hidden variables that preset the value of a physical observable. For example, let us assume that there is a set of unobservable variables that determines precisely what values the position and the momentum of the particle will have at any given time. Although we cannot measure the values of both the momentum and the position precisely, the hidden variables would tell us precisely what the position and the momentum of the particle are at any given time if we were able to read them. Each value of x corresponds to a specific set of values of the hidden variables and, as a result, the collection of all values of the hidden variables can be regarded as a set of distinct and clearly defined subensembles. Below it is argued that such an arrangement is not consistent with quantum-mechanical interference, specifically as applied to that of one particle.

To understand the failings of the hidden-variable theory and the necessity of concluding that quantum-mechanical uncertainty is fundamental, let us consider the following experiment. In optics there is an experiment called Young's experiment or the two-slit experiment. The experimental arrangement consists of a sheet in which two slits are cut. Light is shone incident upon the surface, and the transmitted beam falls onto a screen set up behind the surface, as shown in Figure 1.1.1. The resulting interference pattern attained resembles that sketched in Figure 1.1.2.a. There is a central maximum of light intensity surrounded by a minimum on either side. Arranged around the central maximum are different maxima of varying intensity, as shown in the diagram. As can be clearly seen, the interference pattern illustrates that total cancellation of the intensity occurs at different locations across the screen. Owing to the fact that the beams of light emerging from the two different slits have

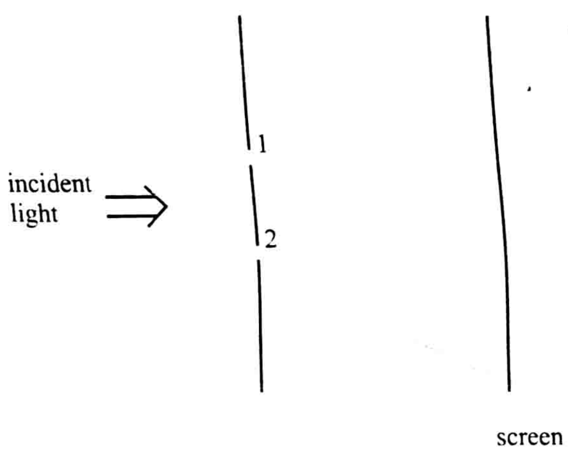

Figure 1.1.1. Schematic diagram of the two-slit experiment.