Electronic Properties of Materials

Fourth Edition

Rolf E. Hummel

Electronic Properties of Materials

Fourth Edition



Rolf E. Hummel College of Engineering University of Florida Rhines Hall 216 Gainesville, FL 32611, USA rhumm@mse.ufl.edu

ISBN 978-1-4419-8163-9 e-ISBN 978-1-4419-8164-6 DOI 10.1007/978-1-4419-8164-6 Springer New York Dordrecht Heidelberg London

Library of Congress Control Number: 2011921720

© Springer Science+Business Media, LLC 2011, 2001, 1993, 1985

All rights reserved. This work may not be translated or copied in whole or in part without the written permission of the publisher (Springer Science+Business Media, LLC, 233 Spring Street, New York, NY 10013, USA), except for brief excerpts in connection with reviews or scholarly analysis. Use in connection with any form of information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed is forbidden. The use in this publication of trade names, trademarks, service marks, and similar terms, even if they are not identified as such, is not to be taken as an expression of opinion as to whether or not they are subject to proprietary rights.

Printed on acid-free paper

(Corrected at 2nd printing 2012)

Springer is part of Springer Science+Business Media (www.springer.com)

Preface to the Fourth Edition

The present textbook, which introduces my readers to elements of solid state physics and then moves on to the presentation of electrical, optical, magnetic, and thermal properties of materials, has been in print for 25 years, i.e. since 1985 when the first edition appeared. It has received quite favorable acceptance by students, professors, and scientists who particularly appreciated that the text is easy to understand and that it emphasizes concepts rather than overburdening the reader with mathematical formalism. I am grateful for all the kind comments which reached me either by personal letters or in reviews found in scientific journals and on the internet.

The third edition was published in 2001, and was followed by a revised printing in 2005. My publisher therefore felt that a new edition would be in order at this time to give me the opportunity to update the material in a field which undergoes explosive development. I do this update with some reluctance because each new edition increases the size (and unfortunately also the price) of a book. It is not my goal to present an encyclopedia on the electronic properties of materials. I still feel that the book should contain just the right amount of material that can be conveniently covered in a 15-week/3-credit hour course. Thus, the added material was restricted to the newest developments in the field. This implies that the fundamentals, particularly in Part I and at the beginning of Parts II to V, remained essentially untouched. However, new topics have been added in the "applied sections", such as energy-saving light sources, particularly compact fluorescence light fixtures, organic light-emitting diodes (OLEDs), organic photovoltaics (OPV cells), optical fibers, pyroelectricity, phase-change memories, blue-ray disks, holographic versatile disks, galvanoelectric phenomena (emphasizing the entire spectrum of primary and rechargeable batteries), graphene, quantum Hall effect, iron-based semiconductors (pnictides), etc., to mention just a few subjects. The reader should find them interesting and educational.

As usual, a book of this wide variety of topics needs the advice of a number of colleagues. I am grateful for the help of Drs. Paul Holloway, Wolfgang Sigmund, Jiangeng Xue, Franky So, Jacob Jones, Thierry Dubroca, all of the University of Florida, Dr. Markus Rettenmayr (Friedrich-Schiller-Universität Jena, Germany), and to Grif Wise.

Gainesville, Florida September 2010

Preface to the Third Edition

Books are seldom finished. At best, they are abandoned. The second edition of "Electronic Properties of Materials" has been in use now for about seven years. During this time my publisher gave me ample opportunities to update and improve the text whenever the book was reprinted. There were about six of these reprinting cycles. Eventually, however, it became clear that substantially more new material had to be added to account for the stormy developments which occurred in the field of electrical, optical, and magnetic materials. In particular, expanded sections on flat-panel displays (liquid crystals, electroluminescence devices, field emission displays, and plasma displays) were added. Further, the recent developments in blue- and greenemitting LED's and in photonics are included. Magnetic storage devices also underwent rapid development. Thus, magneto-optical memories, magneto-resistance devices, and new magnetic materials needed to be covered. The sections on dielectric properties, ferroelectricity, piezoelectricity, electrostriction, and thermoelectric properties have been expanded. Of course, the entire text was critically reviewed, updated, and improved. However, the most extensive change I undertook was the conversion of all equations to SI-units throughout. In most of the world and in virtually all of the international scientific journals use of this system of units is required. If today's students do not learn to utilize it, another generation is "lost" on this matter. In other words, it is important that students become comfortable with SI units.

If plagiarism is the highest form of flattery, then I have indeed been flattered. Substantial portions of the first edition have made up verbatim most of another text by a professor in Madras without giving credit to where it first appeared. In addition, pirated copies of the first and second editions have surfaced in Asian countries. Further, a translation into Korean appeared. Of course, I feel that one should respect the rights of the owner of intellectual property.

I am grateful for the many favorable comments and suggestions promulgated by professors and students from the University of Florida and other schools who helped to improve the text. Dr. H. Rüfer from Wacker Siltronic AG has again appraised me of many recent developments in wafer fabrication. Professor John Reynolds (University of Florida) educated me on the current trends in conducting polymers. Drs. Regina and Gerd Müller (Agilent Corporation) enlightened me on recent LED developments. Professor Paul Holloway (University of Florida) shared with me some insights in phosphors and flat-panel displays. Professor Volkmar Gerold (MPI Stuttgart) was always available when help was needed. My thanks go to all of them.

Gainesville, Florida October 2000

Preface to the Second Edition

It is quite satisfying for an author to learn that his brainchild has been favorably accepted by students as well as by professors and thus seems to serve some useful purpose. This horizontally integrated text on the electronic properties of metals, alloys, semiconductors, insulators, ceramics, and polymeric materials has been adopted by many universities in the United States as well as abroad, probably because of the relative ease with which the material can be understood. The book has now gone through several reprinting cycles (among them a few pirate prints in Asian countries). I am grateful to all readers for their acceptance and for the many encouraging comments which have been received.

I have thought very carefully about possible changes for the second edition. There is, of course, always room for improvement. Thus, some rewording, deletions, and additions have been made here and there. I withstood, however, the temptation to expand considerably the book by adding completely new subjects. Nevertheless, a few pages on recent developments needed to be inserted. Among them are, naturally, the discussion of ceramic (high-temperature) superconductors, and certain elements of the rapidly expanding field of optoelectronics. Further, I felt that the readers might be interested in learning some more practical applications which result from the physical concepts which have been treated here. Thus, the second edition describes common types of field-effect transistors (such as JFET, MOSFET, and MESFET), quantum semiconductor devices, electrical memories (such as D-RAM, S-RAM, and electrically erasable-programmable read-only memories), and logic circuits for computers. The reader will also find an expansion of the chapter on semiconductor device fabrication. The principal mechanisms behind some consumer devices, such as xerography, compact disc players, and optical computers, are also discussed.

Part III (Magnetic Properties of Materials) has been expanded to include more details on magnetic domains, as well as magnetostriction, amorphous ferromagnetics, the newest developments in permanent magnets, new magnetic recording materials, and magneto-optical memories.

Whenever appropriate, some economic facts pertaining to the manufacturing processes or sales figures have been given. Responding to occasional requests, the solutions for the numerical problems are now contained in the Appendix.

I am grateful for valuable expert advice from a number of colleagues, such as Professor Volkmar Gerold, Dr. Dieter Hagmann, Dr. H. Rüfer, Mr. David Malone, Professor Chris Batich, Professor Rolf Haase, Professor Robert Park, Professor Rajiv Singh, and Professor Ken Watson. Mrs. Angelika Hagmann and, to a lesser extent, my daughter, Sirka Hummel, have drawn the new figures. I thank them for their patience.

Gainesville, Florida 1993

Preface to the First Edition

Die meisten Grundideen der Wissenschaft sind an sich einfach und lassen sich in der Regel in einer für jedermann verständlichen Sprache wiedergeben.

-Albert Einstein

The present book on electrical, optical, magnetic, and thermal properties of materials is, in many aspects, different from other introductory texts in solid state physics. First of all, this book is written for engineers, particularly materials and electrical engineers who want to gain a fundamental understanding of semiconductor devices, magnetic materials, lasers, alloys, etc. Second, it stresses concepts rather than mathematical formalism, which should make the presentation relatively easy to understand. Thus, this book provides a thorough preparation for advanced texts, monographs, or specialized journal articles. Third, this book is not an encyclopedia. The selection of topics is restricted to material which is considered to be essential and which can be covered in a 15-week semester course. For those professors who want to teach a two-semester course, supplemental topics can be found which deepen the understanding. (These sections are marked by an asterisk [*].) Fourth, the present text leaves the teaching of crystallography, X-ray diffraction, diffusion, lattice defects, etc., to those courses which specialize in these subjects. As a rule, engineering students learn this material at the beginning of their upper division curriculum. The reader is, however, reminded of some of these topics whenever the need arises. Fifth, this book is distinctly divided into five self-contained parts which may be read independently. All are based on the first part, entitled "Fundamentals of Electron Theory", because the electron theory of materials is a basic tool with which most material properties can be understood. The modern electron theory of solids is relatively involved. It is, however, not my intent to train a student to become proficient in the entire field of quantum theory. This should be left to more specialized texts. Instead, the essential quantum mechanical concepts are introduced only to the extent to which they are needed for the understanding of materials science. Sixth, plenty of practical applications are presented in the text, as well as in the problem sections, so that the students may gain an understanding of many devices that are used every day. In other words, I tried to bridge the gap between physics and engineering. Finally, I gave the treatment of the optical properties of materials about equal coverage to that of the electrical properties. This is partly due to my personal inclinations and partly because it is felt that a more detailed description of the optical properties is needed since most other texts on solid state physics devote relatively little space to this topic. It should be kept in mind that the optical properties have gained an increasing amount of attention in recent years, because of their potential application in communication devices as well as their contributions to the understanding of the electronic structure of materials.

The philosophy and substance of the present text emerged from lecture notes which I accumulated during more than twenty years of teaching. A preliminary version of Parts I and II appeared several years ago in *Journal of Educational Modules for Materials Science and Engineering* **4**, 1 (1982) and **4**, 781 (1982).

I sincerely hope that students who read and work with this book will enjoy, as much as I, the journey through the fascinating field of the physical properties of materials.

Each work benefits greatly from the interaction between author and colleagues or students. I am grateful in particular to Professor R.T. DeHoff, who read the entire manuscript and who helped with his inquisitive mind to clarify many points in the presentation. Professor Ken Watson read the part dealing with magnetism and made many helpful suggestions. Other colleagues to whom I am indebted are Professor Fred Lindholm, Professor Terry Orlando, and Dr. Siegfried Hofmann. My daughter, Sirka Hummel, contributed with her skills as an artist. Last, but not least, I am obliged to my family, to faculty, and to the chairman of the Department of Materials Science and Engineering at the University of Florida for providing the harmonious atmosphere which is of the utmost necessity for being creative.

Gainesville, Florida 1985

Contents

Preface to the Fourth Edition	v
Preface to the Third Edition	vii
Preface to the Second Edition	ix
Preface to the First Edition	xi
PART I	
Fundamentals of Electron Theory	
CHAPTER 1	
Introduction	3
CHAPTER 2	
The Wave-Particle Duality	7
Problems	14
CHAPTER 3	
The Schrödinger Equation	15
3.1. The Time-Independent Schrödinger Equation	15
*3.2. The Time-Dependent Schrödinger Equation	16
*3.3. Special Properties of Vibrational Problems	17
Problems	18
CHAPTER 4	
Solution of the Schrödinger Equation for Four Specific Problems	19
4.1. Free Electrons	19
4.2. Electron in a Potential Well (Bound Electron)	21

Contents	
----------	--

4.3.	Finite Potential Barrier (Tunnel Effect)	25
4.4.	Electron in a Periodic Field of a Crystal (The Solid State)	29
Prob	lems	36

CHAPTER 5 Energy Bands in Crystals 37 37 5.1. One-Dimensional Zone Schemes 5.2. One- and Two-Dimensional Brillouin Zones 42 *5.3. Three-Dimensional Brillouin Zones 45 *5.4. Wigner-Seitz Cells 46 *5.5. Translation Vectors and the Reciprocal Lattice 48 *5.6. Free Electron Bands 52 5.7. Band Structures for Some Metals and Semiconductors 56 5.8. Curves and Planes of Equal Energy 59 Problems 61

CHAPTER 6

Electrons in a Crystal		63
6.1.	Fermi Energy and Fermi Surface	63
6.2.	Fermi Distribution Function	64
6.3.	Density of States	65
6.4.	Complete Density of States Function Within a Band	67
6.5.	Population Density	68
6.6.	Consequences of the Band Model	70
6.7.	Effective Mass	71
6.8.	Conclusion	74
Problems		74
Suggestions for Further Reading (Part I)		75

PART II Electrical Properties of Materials

CHAPTER 7 79 **Electrical Conduction in Metals and Alloys** 79 7.1. Introduction 7.2. Survey 80 7.3. Conductivity-Classical Electron Theory 82 7.4. Conductivity—Quantum Mechanical Considerations 85 7.5. Experimental Results and Their Interpretation 89 7.5.1. Pure Metals 89 7.5.2. Alloys 90 7.5.3. Ordering 92 93 7.6. Superconductivity 7.6.1. Experimental Results 95 *7.6.2. Theory 100

7.7.	Thermoelectric Phenomena	103
7.8.	Galvanoelectric Phenomena (Batteries)	105
	7.8.1. Primary Cells	105
	7.8.2. Secondary Cells	108
	7.8.3. Closing Remarks	112
Prob	blems	113

CHA	PTER 8	
Semi	conductors	115
8.1.	Band Structure	115
8.2.	Intrinsic Semiconductors	117
8.3.	Extrinsic Semiconductors	122
	8.3.1. Donors and Acceptors	122
	8.3.2. Band Structure	123
	8.3.3. Temperature Dependence of the Number of Carriers	124
	8.3.4. Conductivity	125
	8.3.5. Fermi Energy	126
*8.4.	Effective Mass	127
8.5.	Hall Effect	127
8.6.	Compound Semiconductors	129
8.7.	Semiconductor Devices	131
	8.7.1. Metal–Semiconductor Contacts	131
	8.7.2. Rectifying Contacts (Schottky Barrier Contacts)	132
	8.7.3. Ohmic Contacts (Metallizations)	136
	8.7.4. $p-n$ Rectifier (Diode)	137
	8.7.5. Zener Diode	140
	8.7.6. Solar Cell (Photodiode)	141
	*8.7.7. Avalanche Photodiode	145
	*8.7.8. Tunnel Diode	145
	8.7.9. Transistors	147
	*8.7.10. Quantum Semiconductor Devices	156
	8.7.11. Semiconductor Device Fabrication	159
	*8.7.12. Digital Circuits and Memory Devices	168
Proble	ems	177

Problems

101
181
181
191
194
196
200
202
206
210
210

PART III Optical Properties of Materials

CHA	PTER 10	
The (Optical Constants	215
10.1.	Introduction	215
10.2.	Index of Refraction, n	217
10.3.	Damping Constant, k	218
10.4.	Characteristic Penetration Depth, W , and Absorbance, α	222
10.5.	Reflectivity, R, and Transmittance, T	223
10.6.	Hagen–Rubens Relation	225
Proble	ems	225

CHAP	TER 11	
Atomis	stic Theory of the Optical Properties	227
11.1.	Survey	227
11.2.	Free Electrons Without Damping	230
11.3.	Free Electrons With Damping (Classical Free Electron Theory of Metals)	233
11.4.	Special Cases	236
11.5.	Reflectivity	237
11.6.	Bound Electrons (Classical Electron Theory of Dielectric Materials)	238
*11.7.	Discussion of the Lorentz Equations for Special Cases	242
	11.7.1. High Frequencies	242
	11.7.2. Small Damping	242
	11.7.3. Absorption Near v_0	243
	11.7.4. More Than One Oscillator	243
11.8.	Contributions of Free Electrons and Harmonic Oscillators	
	to the Optical Constants	244
Problem	15	245

CHAPTER 12

Quantum Mechanical Treatment of the Optical Properties		247
12.1.	Introduction	247
12.2.	Absorption of Light by Interband and Intraband Transitions	247
12.3.	Optical Spectra of Materials	251
*12.4.	Dispersion	251
Problem	Problems	

CHAP	TER 13	
Applic	ations	259
13.1.	Measurement of the Optical Properties	259
	*13.1.1. Kramers–Kronig Analysis (Dispersion Relations)	260
	*13.1.2. Spectroscopic Ellipsometry	260
	*13.1.3. Differential Reflectometry	263
13.2.	Optical Spectra of Pure Metals	266
	13.2.1. Reflection Spectra	266
	*13.2.2. Plasma Oscillations	270

13.3.	Optical Spectra of Alloys	271
*13.4.	Ordering	275
*13.5.	Corrosion	277
13.6.	Semiconductors	278
13.7.	Insulators (Dielectric Materials and Glass Fibers)	281
13.8.	Emission of Light	284
	13.8.1. Spontaneous Emission	284
	13.8.2. Stimulated Emission (Lasers)	288
	13.8.3. Helium–Neon Laser	291
	13.8.4. Carbon Dioxide Laser	292
	13.8.5. Semiconductor Laser	293
	13.8.6. Direct–Versus Indirect–Band Gap Semiconductor Lasers	295
	13.8.7. Wavelength of Emitted Light	296
	13.8.8. Threshold Current Density	297
	13.8.9. Homojunction Versus Heterojunction Lasers	298
	13.8.10. Laser Modulation	299
	13.8.11. Laser Amplifier	300
	13.8.12. Quantum Well Lasers	301
	13.8.13. Light-Emitting Diodes (LED)	302
	13.8.14. Organic Light Emitting Diodes (OLEDs)	305
	13.8.15. Organic Photovoltaic Cells (OPVCs)	308
	13.8.16. Liquid Crystal Displays (LCDs)	310
	13.8.17. Emissive Flat-Panel Displays	312
13.9.	Integrated Optoelectronics	315
	13.9.1. Passive Waveguides	315
	13.9.2. Electro-Optical Waveguides (EOW)	317
	13.9.3. Optical Modulators and Switches	319
	13.9.4. Coupling and Device Integration	320
	13.9.5. Energy Losses	322
	13.9.6. Photonics	323
	13.9.7. Optical Fibers	324
13.10.	Optical Storage Devices	325
13.11.	The Optical Computer	329
13.12.	X-Ray Emission	332
Proble	ms	334
Sugges	stions for Further Reading (Part III)	335

PART IV

Magnetic Properties of Materials

CHAPTER 14

Foundations of Magnetism		339
14.1.	Introduction	339
14.2.	Basic Concepts in Magnetism	340
*14.3.	Units	344
Problems		345

CHAPTER 15

Magne	tic Phenomena and Their Interpretation—Classical Approach	347
15.1.	Overview	347
	15.1.1. Diamagnetism	347
	15.1.2. Paramagnetism	349
	15.1.3. Ferromagnetism	352
	15.1.4. Antiferromagnetism	358
	15.1.5. Ferrimagnetism	359
15.2.	Langevin Theory of Diamagnetism	362
*15.3.	Langevin Theory of (Electron Orbit) Paramagnetism	364
*15.4.	Molecular Field Theory	368
Problen	15	371

CHAPTER 16

Quantum Mechanical Considerations		373
16.1.	Paramagnetism and Diamagnetism	373
16.2.	Ferromagnetism and Antiferromagnetism	378
Problems		382

CHAPTER 17	
Applications	385
17.1. Introduction	385
17.2. Electrical Steels (Soft Magnetic Materials)	385
17.2.1. Core Losses	386
17.2.2. Grain Orientation	388
17.2.3. Composition of Core Materials	390
17.2.4. Amorphous Ferromagnets	390
17.3. Permanent Magnets (Hard Magnetic Materials)	391
17.4. Magnetic Recording and Magnetic Memories	394
17.4.1. Closing Remarks	400
Problems	400
Suggestions for Further Reading (Part IV)	

PART V

Thermal Properties of Materials

CHAPTER 18 Introduction	405
CHAPTER 19	
Fundamentals of Thermal Properties	409
19.1. Heat, Work, and Energy	409
19.2. Heat Capacity, C'	410
19.3. Specific Heat Capacity, c	411
19.4. Molar Heat Capacity, C_v	412

19.5.	Thermal Conductivity, K	413
19.6.	The Ideal Gas Equation	414
19.7.	Kinetic Energy of Gases	415
Problems		416

CHA	PTER 20	
Heat	Capacity	419
20.1.	Classical (Atomistic) Theory of Heat Capacity	419
20.2.	Quantum Mechanical Considerations—The Phonon	421
	20.2.1. Einstein Model	421
	20.2.2. Debye Model	424
20.3.	Electronic Contribution to the Heat Capacity	426
Proble	ems	429

CHAPTER 21

nal Conduction	431
Thermal Conduction in Metals and Alloys-Classical Approach	432
Thermal Conduction in Metals and Alloys—Quantum	
Mechanical Considerations	434
Thermal Conduction in Dielectric Materials	435
ms	437
1	nal Conduction Thermal Conduction in Metals and Alloys—Classical Approach Thermal Conduction in Metals and Alloys—Quantum Mechanical Considerations Thermal Conduction in Dielectric Materials ms

CHAPTER 22

Thermal Expansion Problems Suggestions for Further Reading (Part V)		439 441
		Appen
App. 1.	Periodic Disturbances	445
App. 2.	Euler Equations	450
App. 3.	Summary of Quantum Number Characteristics	451
App. 4.	Tables	454
App. 5.	About Solving Problems and Solutions to Problems	467
About the Author		473
Index		475

Note: Sections marked with an asterisk (*) are topics which are beyond a 15-week semester course or may be treated in a graduate course.