

Springer Tracts in Modern Physics

Volume 271

Series Editors

Yan Chen, Department of Physics, Fudan University, Shanghai, China

Atsushi Fujimori, Department of Physics, University of Tokyo, Tokyo, Japan

William C. Stwalley, Department of Physics, University of Connecticut, Storrs,
USA

Jianke Yang, Department of Mathematics and Statistics, University of Vermont,
Burlington, VT, USA

Springer Tracts in Modern Physics provides comprehensive and critical reviews of topics of current interest in physics. The following fields are emphasized:

- Elementary Particle Physics
- Condensed Matter Physics
- Light Matter Interaction
- Atomic and Molecular Physics
- Complex Systems
- Fundamental Astrophysics

Suitable reviews of other fields can also be accepted. The Editors encourage prospective authors to correspond with them in advance of submitting a manuscript. For reviews of topics belonging to the above mentioned fields, they should address the responsible Editor as listed in “Contact the Editors”.

More information about this series at <http://www.springer.com/series/426>

Maurizio Dapor

Transport of Energetic Electrons in Solids

Computer Simulation with Applications
to Materials Analysis and Characterization

Third Edition

 Springer

Maurizio Dapor
European Centre for Theoretical Studies
in Nuclear Physics and Related Areas
Trento, Italy

ISSN 0081-3869 ISSN 1615-0430 (electronic)
Springer Tracts in Modern Physics
ISBN 978-3-030-43263-8 ISBN 978-3-030-43264-5 (eBook)
<https://doi.org/10.1007/978-3-030-43264-5>

1st edition: © Springer International Publishing Switzerland 2014

2nd edition: © Springer International Publishing AG 2017

3rd edition: © Springer Nature Switzerland AG 2020

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, expressed or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Switzerland AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

*To my dearest father, always alive in my mind
and in my heart*

Preface to the Third Edition

This volume is an extended edition of a book published in 2014 (first edition) and 2017 (second edition). It provides all the information necessary to the reader to write his/her own Monte Carlo code. The possibility to compare the obtained results with the many numerical and experimental examples presented through the text can help the reader to better describe and understand the processes and the phenomena concerning the transport of electrons and positrons in solid targets.

The updated content of this third edition includes the theory of the spin-polarized electron beams, the study of elastic scattering by molecules, a simple derivation of the Bethe-Bloch stopping power formula, the f-sum rule and the ps-sum rule, the Vicanek and Urbassek formula for the calculation of the backscattering coefficient, and the Wolff theory of the secondary electron spectra.

A new chapter is devoted to the basic concepts of computational physics. Another chapter is dedicated to the elementary aspects of the interaction of beams of electrons and positrons with thin solid films (the so-called multiple reflection method).

Further comparisons between theory and experimental data are presented here as well.

Villazzano, Italy

Maurizio Dapor

Preface to the Second Edition

This book describes all the mechanisms of scattering (elastic and inelastic) of electrons with the atoms of the target in the simplest possible way. The use of techniques of quantum mechanics is described in detail for the investigation of interaction processes of electrons with matter. The book presents the strategies of the Monte Carlo method, as well as numerous comparisons among the results of the simulations with the experimental data available in the literature. The new content of this extended and updated second edition includes the derivation of the Rutherford formula, details about the calculation of the phase shifts that are used in the relativistic partial wave expansion method, and the description of the Mermin theory. The role of secondary electrons in the proton cancer therapy is discussed as well in the chapter devoted to applications: in this context, Monte Carlo results about the radial distribution of the energy deposited in solids by secondary electrons generated by energetic proton beams are presented.

Povo, Italy
August 2016

Maurizio Dapor

Preface to the First Edition

In modern physics, we are interested in systems with many degrees of freedom. Let us consider, for example, the number of atoms in a solid, the number of electrons in an atom, or the number of electrons of a beam interacting with the many atoms and electrons of a solid.

In many situations, these systems can be described by the calculations of definite integrals of very high dimension. An example is the evaluation of the classical partition function for a gas of many atoms at a temperature T . The Monte Carlo method gives us a very accurate way to calculate high-dimensional definite integrals: it evaluates the integrand at a random sampling of abscissa.

The Monte Carlo method is also used for evaluating many physical quantities necessary for the study of the interactions of particle beams with solid targets. The simulation of the involved physical processes, by random sampling, allows to solve many particle transport problems. Letting the particles carry out an artificial, random walk—taking into account the effect of the single collisions—it is possible to accurately evaluate the diffusion process.

This book is devoted to the electron beam interactions with the solid targets. As a researcher in this field, I am persuaded that a book on kV electron transport in solids can be very useful. It is difficult, for the newcomer, to find this topic exhaustively treated; and it is not easy for the beginner to sort out the importance of the great number of published papers.

The Monte Carlo simulation is the most powerful theoretical method for evaluating the physical quantities related to the interaction of electrons with a solid target. A Monte Carlo simulation can be considered as an idealized experiment. The simulation does not investigate the fundamental principles of the interaction. It is necessary to know them—in particular the energy loss and angular deflection phenomena—to produce a good simulation.

This book is complementary with respect to many other texts dedicated to similar subjects (including my book entitled *Electron-Beam Interactions with Solids*, published by Springer-Verlag in 2003) for the following two aspects.

1. I have, on the one hand, systematically minimized the mathematical contents of the more difficult theoretical parts. Since the essential concept to digest is the meaning of the various cross sections, the mathematical details, for the sake of clarity, have been deliberately avoided. I have reduced the theoretical part to the presentation of the energy loss and the angular deflections, providing simple recipes to calculate the stopping power, the differential inverse inelastic mean free path, and the differential elastic scattering cross section. This allowed me to avoid to describe in depth quantum theory. Mathematical contents and details can be found in the Appendices, in my previous book, and in many other books dedicated to modern physics and quantum mechanics.
2. In the derivation and use of the simpler theoretical transport models, I have, on the other hand, included many details. I think, indeed, there is a need for a basic physical picture in order to provide the beginner with a solid background about electron transport in solids. This can be only achieved by a step-by-step derivation of the analytical formulas.

Comparing available experimental data with simulation results is a fundamental step in evaluating the quality of the Monte Carlo codes. Selected applications of the Monte Carlo method to kV electron transport in solids are presented in the second part of this book. The book compares computational simulations and experimental data in order to offer a more global vision.

Povo, Italy
October 2013

Maurizio Dapor

Acknowledgements

I would like to gratefully thank my beloved children for their immense patience and words of encouragement.

I am grateful to my dear parents for their great affection and love.

I wish to express warm gratitude to my cherished Roberta for always being supportive.

It is also a pleasure to mention many people, friends, and colleagues who, with their enthusiasm, invaluable suggestions, ideas, and competence, considerably contributed to achieve the results presented in this book: I am, in particular, very grateful to Diego Bisero, Lucia Calliari, Giovanni Garberoglio, Simone Taioli, and Paolo Emilio Trevisanutto for their help and sincere friendship.

I am also indebted to all the researchers who made possible, with their help, the completion of the project: Kerry J. Abrams, Isabel Abril, Martina Azzolini, Nicola Bazzanella, Mauro Borghesi, Eric Bosch, Mauro Ciappa, Michele Crivellari, Pablo de Vera, Sergey Fanchenko, Wolfgang Fichtner, Massimiliano Filippi, Jan Franz, Małgorzata Franz, Rafael Garcia-Molina, Stefano Gialanella, Stephan Holzer, Emre Ilgüsatiroglu, Beverley J. Inkson, Mark A. E. Jepson, Alexander Koschik, Robert C. Masters, Antonio Miotello, Tommaso Morresi, Francesco Pederiva, Andrea Pedrielli, Nicoletta Plotegher, Maciej Polak, Cornelia Rodenburg, John M. Rodenburg, Manoranjan Sarkar, Paolo Scardi, Giorgina Scarduelli, Siegfried Schmauder, Emanuele Scifoni, Stefano Simonucci, Nicola Stehling, Laura Toniutti, Chia-Kuang (Frank) Tsung, Jochen Wambach, Quan Wan, and Wolfram Weise.

I also wish to express my sincere gratitude to all the students of my course entitled Computational Methods for Transport Phenomena (Department of Physics, University of Trento) for their kind questions, their clever suggestions, and their excellent and illuminating ideas.

I would like to thank all my colleagues at the Interdisciplinary Laboratory for Computational Science (LISC) in Trento for the fruitful discussions. The stimulating atmosphere of LISC provided the ideal environment to work on this project.

I am grateful to Maria Del Huerto Flammia for assisting me with the proof-reading of this book.

I acknowledge the support of the Leverhulme Trust through the Visiting Professorship VP1-2014-011 (Department of Engineering Materials of the University of Sheffield).

I wish also to thank the European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT*), the Fondazione Bruno Kessler (FBK), the Trento Institute for Fundamentals Physics and Applications (TIFPA), the Department of Materials Science and Engineering of the University of Sheffield, the Integrated Systems Laboratory of the Swiss Federal Institute of Technology (ETH) of Zurich, and the Departament de Física Aplicada of the Universitat d'Alacant.

Contents

1	Electron Transport in Solids	1
1.1	Motivation: Why Are Electrons Important	1
1.2	The Monte Carlo Method	2
1.3	The Monte Carlo Ingredients	2
1.4	Electron-Beam Interactions with Solids	3
1.5	Electron Energy-Loss Peaks	5
1.6	Auger Electron Peaks	7
1.7	Secondary Electron Peak	7
1.8	Characterization of Materials	8
1.9	Summary	9
	References	9
2	Computational Minimum	11
2.1	Numerical Differentiation	11
2.2	Numerical Quadrature	12
2.2.1	Trapezoidal Rule, Simpson’s Rule, Bode’s Rule	12
2.2.2	Gaussian Quadrature	13
2.3	Ordinary Differential Equations	14
2.4	Special Functions of Mathematical Physics	16
2.4.1	Legendre Polynomials and Associated Legendre Functions	16
2.4.2	Bessel Functions	17
2.5	Summary	19
	References	20
3	Cross-Sections. Basic Aspects	21
3.1	Cross-Section and Probability of Scattering	22
3.2	Stopping Power and Inelastic Mean Free Path	23
3.3	Range	24
3.4	Energy Straggling	25

3.5	Summary	26
	References	26
4	Scattering Mechanisms	27
4.1	Elastic Scattering	28
4.1.1	Mott Cross-Section Versus Screened Rutherford Cross-Section	29
4.1.2	Polarized Electron Beams Elastically Scattered by Atoms	34
4.1.3	Electron-Molecule Elastic Scattering	38
4.2	Quasi-elastic Scattering	40
4.2.1	Electron-Phonon Interaction	40
4.3	Inelastic Scattering	41
4.3.1	Stopping: Bethe-Bloch Formula	41
4.3.2	Stopping: Semi-empiric Formulas	45
4.3.3	Dielectric Theory	45
4.3.4	Sum of Drude Functions	51
4.3.5	The Mermin Theory	54
4.3.6	Exchange Effects	55
4.3.7	Polaronic Effect	56
4.4	Surface Phenomena	57
4.5	Summary	60
	References	60
5	Random Numbers	63
5.1	Generating Pseudo-random Numbers	63
5.2	Testing Pseudo-random Number Generators	64
5.3	Pseudo-random Numbers Distributed According to a Given Probability Density	64
5.4	Pseudo-random Numbers Uniformly Distributed in the Interval $[a, b]$	64
5.5	Pseudo-random Numbers Distributed According to the Exponential Density of Probability	65
5.6	Pseudo-random Numbers Distributed According to the Gauss Density of Probability	66
5.7	Summary	67
	References	68
6	Monte Carlo Strategies	69
6.1	The Continuous-Slowing-Down Approximation	70
6.1.1	The Step-Length	70
6.1.2	Interface Between Over-Layer and Substrate	70
6.1.3	The Polar Scattering Angle	71
6.1.4	Direction of the Electron After the Last Deflection	71
6.1.5	Electron Position in Three Dimensional Cartesian Coordinates	72

6.1.6	The Energy Loss	73
6.1.7	End of the Trajectory and Number of Trajectories	73
6.2	The Energy-Straggling Strategy	73
6.2.1	The Step-Length	74
6.2.2	Elastic and Inelastic Scattering	75
6.2.3	Energy Loss	75
6.2.4	Electron-Atom Collisions: Scattering Angle	76
6.2.5	Electron-Electron Collisions: Scattering Angle	76
6.2.6	Electron-Phonon Collisions: Scattering Angle	78
6.2.7	Direction of the Electron After the Last Deflection	79
6.2.8	The First Step	79
6.2.9	Transmission Coefficient	79
6.2.10	How Inelastic Scattering Depends on the Distance from the Surface	81
6.2.11	End of the Trajectory and Number of Trajectories	83
6.3	Summary	84
	References	84
7	Electron Beam Interactions with Solid Targets and Thin Films. Basic Aspects	85
7.1	Definitions, Symbols, Properties	85
7.2	Unsupported Thin Films	87
7.3	Supported Thin Films	89
7.4	Summary	90
	References	91
8	Backscattering Coefficient	93
8.1	Electrons Backscattered from Bulk Targets	93
8.1.1	The Backscattering Coefficient: An Analytical Model	94
8.1.2	The Backscattering Coefficient: Monte Carlo Simulation	95
8.2	Electrons Backscattered from One Layer Deposited on Semi-infinite Substrates	97
8.2.1	Carbon Overlayers	97
8.2.2	Gold Overlayers	99
8.3	Electrons Backscattered from Two Layers Deposited on Semi-infinite Substrates	100
8.4	A Comparative Study of Electron and Positron Backscattering Coefficients and Depth Distributions	106
8.5	Summary	108
	References	109

- 9 Secondary Electron Yield 111**
 - 9.1 Secondary Electron Emission 112
 - 9.2 Monte Carlo Approaches to the Study of Secondary Electron Emission 112
 - 9.3 Specific MC Methodologies for SE Studies 113
 - 9.3.1 Continuous-Slowing-Down Approximation (CSDA Scheme) 113
 - 9.3.2 Energy-Straggling (ES Scheme) 114
 - 9.4 Secondary Electron Yield: PMMA and Al₂O₃ 115
 - 9.4.1 Secondary Electron Emission Yield as a Function of the Energy 115
 - 9.4.2 Comparison Between ES Scheme and Experiment 115
 - 9.4.3 Comparison Between CSDA Scheme and Experiment 116
 - 9.4.4 CPU Time 117
 - 9.5 Summary 119
 - References 119
- 10 Electron Energy Distributions 121**
 - 10.1 Monte Carlo Simulation of the Spectrum 121
 - 10.2 Plasmon Losses and Electron Energy Loss Spectroscopy 123
 - 10.2.1 Plasmon Losses in Graphite 123
 - 10.2.2 Plasmon Losses in Silicon Dioxide 124
 - 10.3 Energy Losses of Auger Electrons 125
 - 10.4 Elastic Peak Electron Spectroscopy (EPES) 127
 - 10.5 Spectrum of Secondary Electrons 128
 - 10.5.1 Wolff Theory 129
 - 10.5.2 Other Formulas Describing the Spectrum of the Secondary Electrons 133
 - 10.5.3 Initial Polar and Azimuth Angle of the Secondary Electrons 133
 - 10.5.4 Comparison with Theoretical and Experimental Data 134
 - 10.6 Summary 137
 - References 137
- 11 Applications 139**
 - 11.1 Linewidth Measurement in Critical Dimension SEM 139
 - 11.1.1 Critical Dimension SEM 139
 - 11.1.2 Lateral and Depth Distributions 140
 - 11.1.3 Linescan of a Silicon Step 140
 - 11.1.4 Linescan of PMMA Lines on a Silicon Substrate 141
 - 11.2 Application to Energy Selective Scanning Electron Microscopy 142

11.2.1	Doping Contrast	143
11.2.2	Energy Selective Scanning Electron Microscopy	144
11.3	Energy Density Radially Deposited Along Ion Tracks	145
11.3.1	Ion Track Simulation and Bragg Peak	145
11.3.2	Damage in the Biomolecules by Dissociative Electron Attachment	145
11.3.3	Simulation of Electron Transport and Further Generation	146
11.3.4	Radial Distribution of the Energy Deposited in PMMA by Secondary Electrons Generated by Energetic Proton Beams	147
11.4	Summary	147
	References	148
	Appendix A: The First Born Approximation and the Rutherford Cross-Section.	151
	Appendix B: The Mott Theory	159
	Appendix C: The Fröhlich Theory	181
	Appendix D: The Ritchie Theory.	193
	Appendix E: The Chen and Kwei and the Li et al. Theory.	199
	Appendix F: The Mermin Theory and the Generalized Oscillator Strength Method	203
	Appendix G: The Kramers–Kronig Relations and the Sum Rules	207
	Appendix H: From the Electron Energy Loss Spectrum to the Dielectric Function.	215
	Index	217