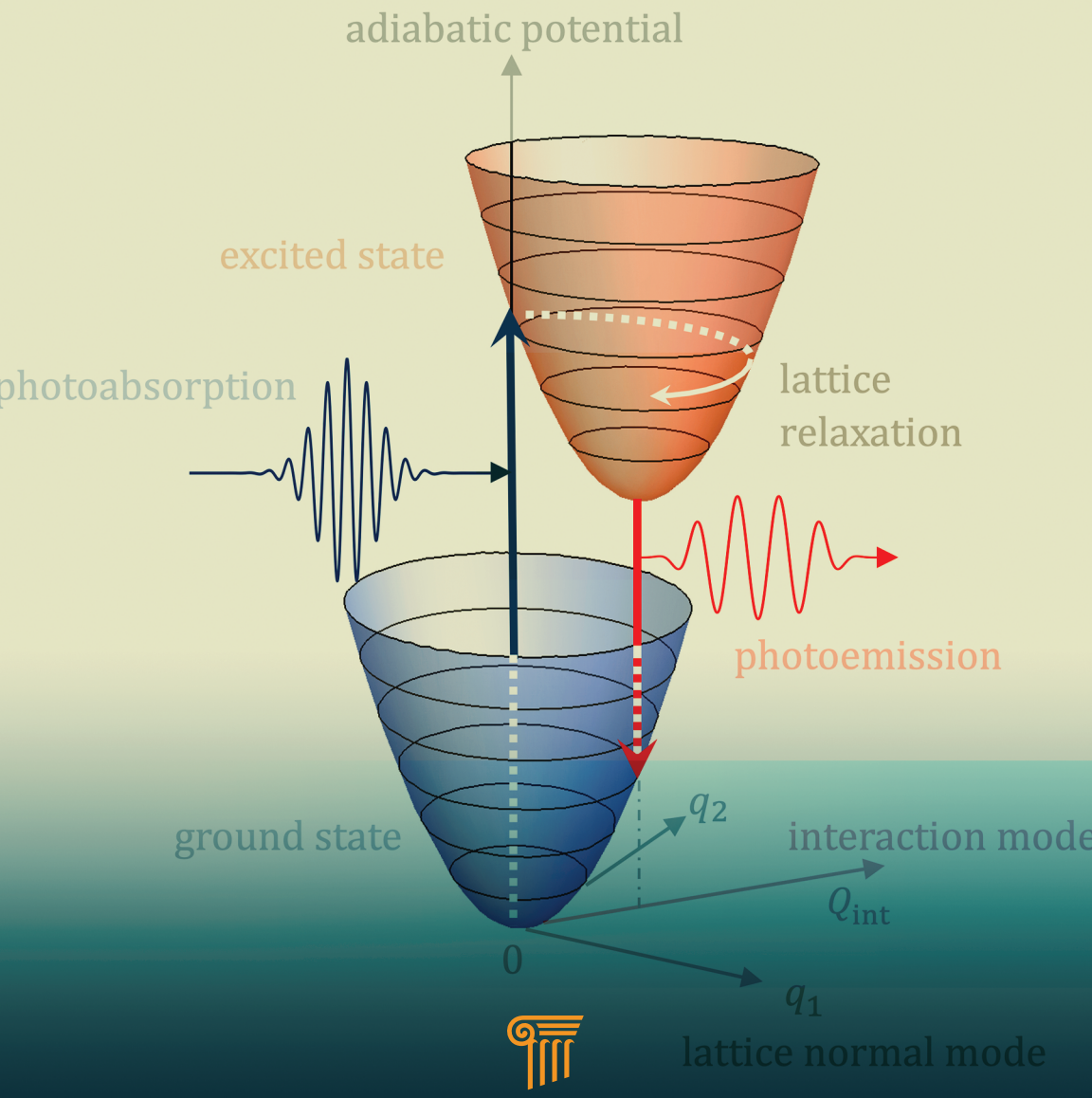
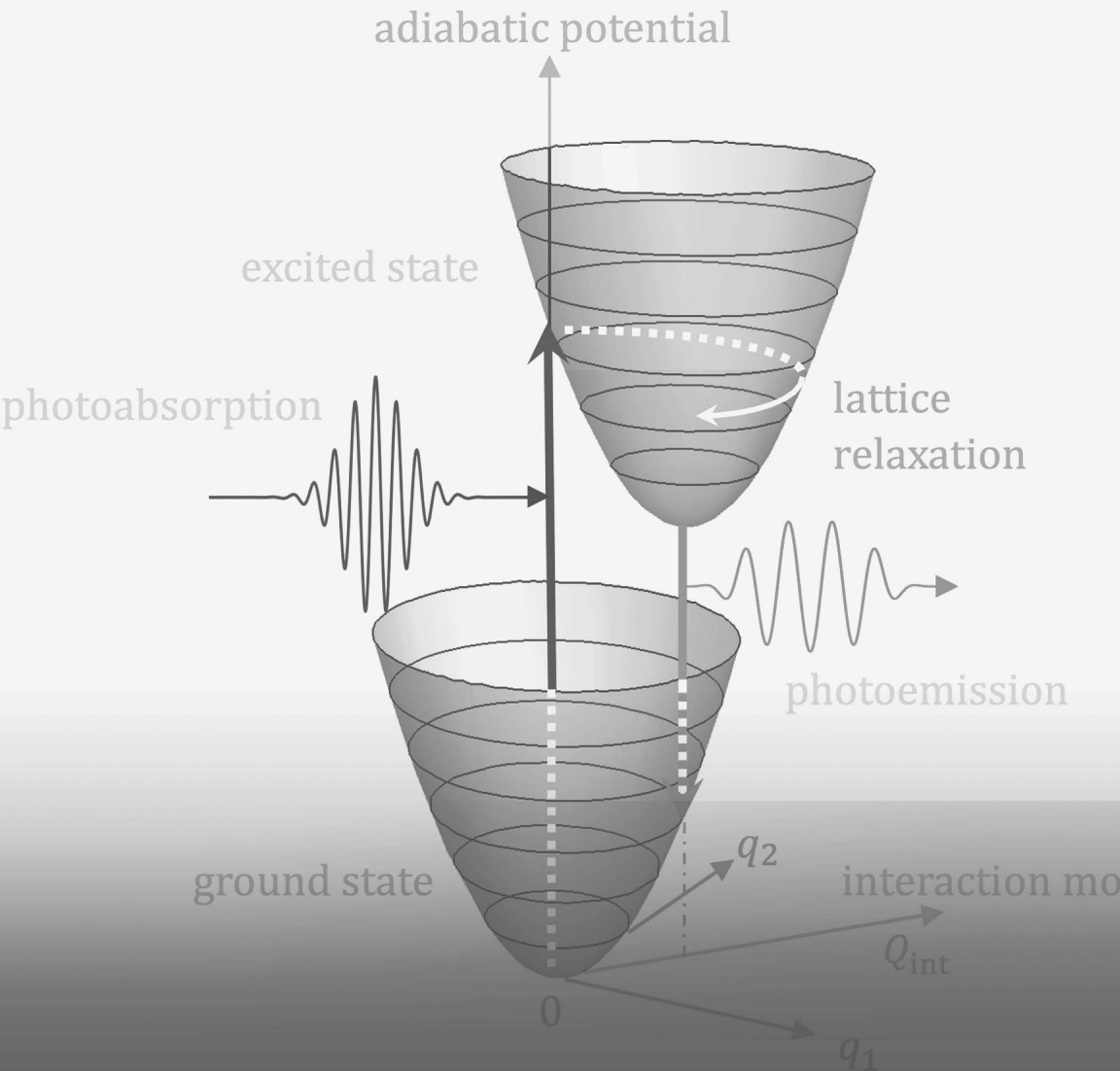
Electron-Lattice Interactions in Semiconductors

Yuzo Shinozuka



Electron-Lattice Interactions in Semiconductors



Electron-Lattice Interactions in Semiconductors

Yuzo Shinozuka

JENNY STANFORD
PUBLISHING

Published by

Jenny Stanford Publishing Pte. Ltd.
Level 34, Centennial Tower
3 Temasek Avenue
Singapore 039190

Email: editorial@jennystanford.com
Web: www.jennystanford.com

British Library Cataloguing-in-Publication Data
A catalogue record for this book is available from the British Library.

Electron–Lattice Interactions in Semiconductors
Copyright © 2021 Jenny Stanford Publishing Pte. Ltd.

All rights reserved. This book, or parts thereof, may not be reproduced in any form or by any means, electronic or mechanical, including photocopying, recording or any information storage and retrieval system now known or to be invented, without written permission from the publisher.

For photocopying of material in this volume, please pay a copying fee through the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, USA. In this case permission to photocopy is not required from the publisher.

ISBN 978-981-4800-96-9 (Hardcover)
ISBN 978-1-003-02346-3 (eBook)

Contents

Preface ix

1. Perfect Crystal **1**

1.1 Basic Hamiltonian 1
1.2 Adiabatic Approximation 3
1.3 Crystal Structures of Bulk Materials 5
1.4 Electronic States in Crystals: Band Theory 8
1.5 Lattice Vibrations in Crystals 12
1.5.1 Lagrangian of the Lattice 12
1.5.2 Dynamics of Ions 14
1.5.3 Lattice Vibration Modes 17
1.5.4 Theoretical Models for Force Constant 18
1.5.5 Note on Electronic States during the Lattice Vibrations 20
1.5.6 Hamiltonian of the Lattice Vibrations 22
1.5.7 Lattice Dynamics: Phonon 23
1.5.8 Thermal Properties of Phonons 25
1.5.9 Specific Heat 25

2. Electron–Lattice Interaction **31**

2.1 Electronic Excited States 31
2.2 Hamiltonian of a Single Carrier 33
2.2.1 A Conduction Electron 33
2.2.2 Effective Hamiltonian for Conduction Electron 36
2.2.3 Effective Hamiltonian for Interaction Part: V_{eL} 39
2.2.4 A Valence Hole 46

2.3 Carrier Scattering 50
2.4 Polaron: Carrier Dressed with Phonons 54
2.4.1 Fröhlich Polaron 54
2.4.2 Polaron by Deformation Potential and Self-Trapping 57

3. Configuration Coordinate Diagram 61

3.1 Adiabatic Instability 61
3.2 CCD for Two-Level System 62
3.3 Lattice Relaxation Dynamics in Two-Level System 65
3.4 Photoabsorption and Photoemission (Classical and Statistical Treatment) 68
3.4.1 Photoabsorption 68
3.4.2 Photoemission (Classical Treatment) 71
3.5 Photoabsorption and Photoemission at a Localized Electron System (Quantum Treatment) 72
3.5.1 Coupled with a Single Lattice Mode 72
3.5.2 Coupled with Many Lattice Modes 76
3.6 Nonradiative Transition 79
3.7 Physics of Relaxation 81

4. Localization: Self-Trapping 85

4.1 Study of Polaron (Self-Trapping) with Continuum Model 85
4.1.1 Perfect Crystal 86
4.1.2 Characterization of Carriers in Non-Metallic Material 91
4.1.3 Isoelectronic Impurity: Extrinsic Self-Trapping 92
4.1.4 Exciton (an Electron–Hole Pair) in the Phonon-Fields 95
4.2 Study of Self-Trapping Using Tight Binding Model 97
4.2.1 Sum Rule on the Lowest (Relaxed) States 98
4.2.2 Homogeneous Pure System 99
4.2.3 Infinite Anisotropic System 102

4.2.4 Quantum Well 103
4.3 Adiabatic Potential Using Tight Binding Model 104
4.3.1 Adiabatic Potential in 3-dim. Crystals 105
4.3.2 Optical Spectra 107
4.3.3 Isoelectric Impurity (Extrinsic Self-Trapping) 107
4.3.4 Alloy Semiconductor (Mixed Crystal) 109
4.4 Characterization of Carriers in Semiconductors 111
4.4.1 Alkali Halides and Ag Halides 112
4.4.2 Impurity 113
4.4.3 Alloy Semiconductor 114
4.5 Small Polaron: Holstein Approach 116

5. Optical Spectra in Perfect Crystals: Final State Interaction 119

5.1 Adiabatic Instability of a Free Electron in a Deformable Lattice 119
5.2 Optical Absorption in Perfect Crystals 123
5.2.1 Urbach–Martiessen Rule 123
5.2.2 Relation with Emission Spectra 127

6. Electron–Lattice Interaction at Deep-Level Defects 129

6.1 Deep-Localized States Couple with Conduction or Valence Band 130
6.1.1 One-Electron Scheme 130
6.1.2 Trapping of a Conduction Electron 130
6.1.2.1 General 130
6.1.2.2 Simple situation 132
6.1.3 Localized Electron Deep into VB: Incorrect CCD 135
6.1.4 Trapping of a Valence Hole 137
6.1.4.1 General 137
6.1.4.2 Simple situation 138
6.2 Deep-Localized States Couple with Valence and Conduction Bands 140
6.2.1 Calculation of Localized State in the Band Gap 140

6.2.2 Adiabatic Potentials 143
6.2.3 Far Deep into the Valence Band 150
6.2.4 CC Diagram for Many Carriers 150
6.2.5 Application to Typical Defects 152
6.2.6 Several Localized Electrons 153

7. Nonradiative Multiphonon Capture and Recombination Processes 157

7.1 Nonradiative Multiphonon Recombination 157
7.1.1 Configuration Coordinate Diagram 158
7.1.2 First Carrier Capture 161
7.1.3 Induced Transient Lattice Vibration 162
7.1.4 Second Capture 162
7.2 Simulation of Successive Captures 165
7.2.1 Model 165
7.2.2 Inflation of Vibration 166
7.2.3 Summary 167

8. Symmetry Breaking Processes 171

8.1 Jahn–Teller Effect 171
8.2 Stability of the Position of an Impurity 175
8.3 Bourgoin–Corbett Mechanism 177
8.4 Tetrahedral T-U-S Model 178

9. Modification of Semiconductors: Destruction and Creation 187

9.1 Return to the Beginning: Condensed Matter 187
9.2 Strong Electron–Lattice Interaction: Defect Process 188
9.3 Phonon-Kick Mechanism for Defect Reactions 190
9.4 Defect Processes 192
9.5 Control the Electron–Lattice Interaction 193
9.6 Expolar Novel Metastructures in the Dark 194

Appendixes 201
Index 237

Preface

This book is for graduate students who have finished the basic study in solid-state physics and also for research scientists and engineers who participate in materials science and engineering, including the research of electronic and optical semiconductor devices. I did not intend to write a second version of ordinary textbooks on semiconductor physics, but I have presented here underlying physics and theoretical treatments not found in usual textbooks. The necessary knowledge is the basic quantum mechanics and solid-state physics. The target readers are those who are interested in the theoretical approach to semiconductor physics, participating in experimental as well as theoretical researches.

The book starts with a description of the basic properties of condensed matter, treating the system as a macroscopic association of electrons and ions. In their ground state, fruitful results are derived on crystal semiconductors, such as the band theory of electrons in a periodic lattice and the lattice vibrations. The electron–lattice interaction is then introduced as a dynamical response of condensed matter when it is electronically excited. Various optical electro-atomic processes are precisely explained with the aid of proper configuration coordinate diagrams, including carrier scattering, polaron formation, lattice relaxation, Stokes shift and phonon side band in optical spectrum, intrinsic and extrinsic self-trapping, multiphonon process of carrier capture, nonradiative recombination, and symmetry-breaking structural changes.

Half of the contents of this book are somewhat differently described from those of other textbooks on semiconductors. I have tried to show and explain various electronic and atomic processes from a unified point of view. Although the book does not contain many calculation methods to obtain the quantitative value of physical parameters in semiconductors, after reading this book, I hope readers will deeply understand the mechanism

of the above-mentioned phenomena, i.e., underlying physics in materials science with fruitful concepts.

This book is dedicated to late Professor Yutaka Toyozawa of the Institute for Solid State Physics, University of Tokyo. He showed me the significance of the optical processes in condensed matter physics and his perspective on the future materials science. Many of the contents in this book are originated from his suggestions and discussion. Special thanks to Professor Keiichiro Nasu and Professor Yosuke Kayanuma for fruitful discussion and sharing their excellent idea in physics since I started my research. I would like to show my greatest appreciation to Professor Koji Maeda and Professor Koichi Murakami for their long-term collaboration in the project "Nano processes by Electronic Excitation" in Japan. Thanks are also due to colleagues and students at Yamaguchi University and Wakayama University for their help, support, and discussion.

I would like to acknowledge all people who have helped me in preparing the manuscript and publishing this book. The support by the JSPS KAKENHI Grant no. JP16H06425 is highly appreciated.

Last but not least, I am very grateful to my wife, Keiko, who assisted me during this time-consuming preparation of the manuscript with great patience and heartful encouragement.

Yuzo Shinozuka
October 7, 2020
Wakayama, Japan