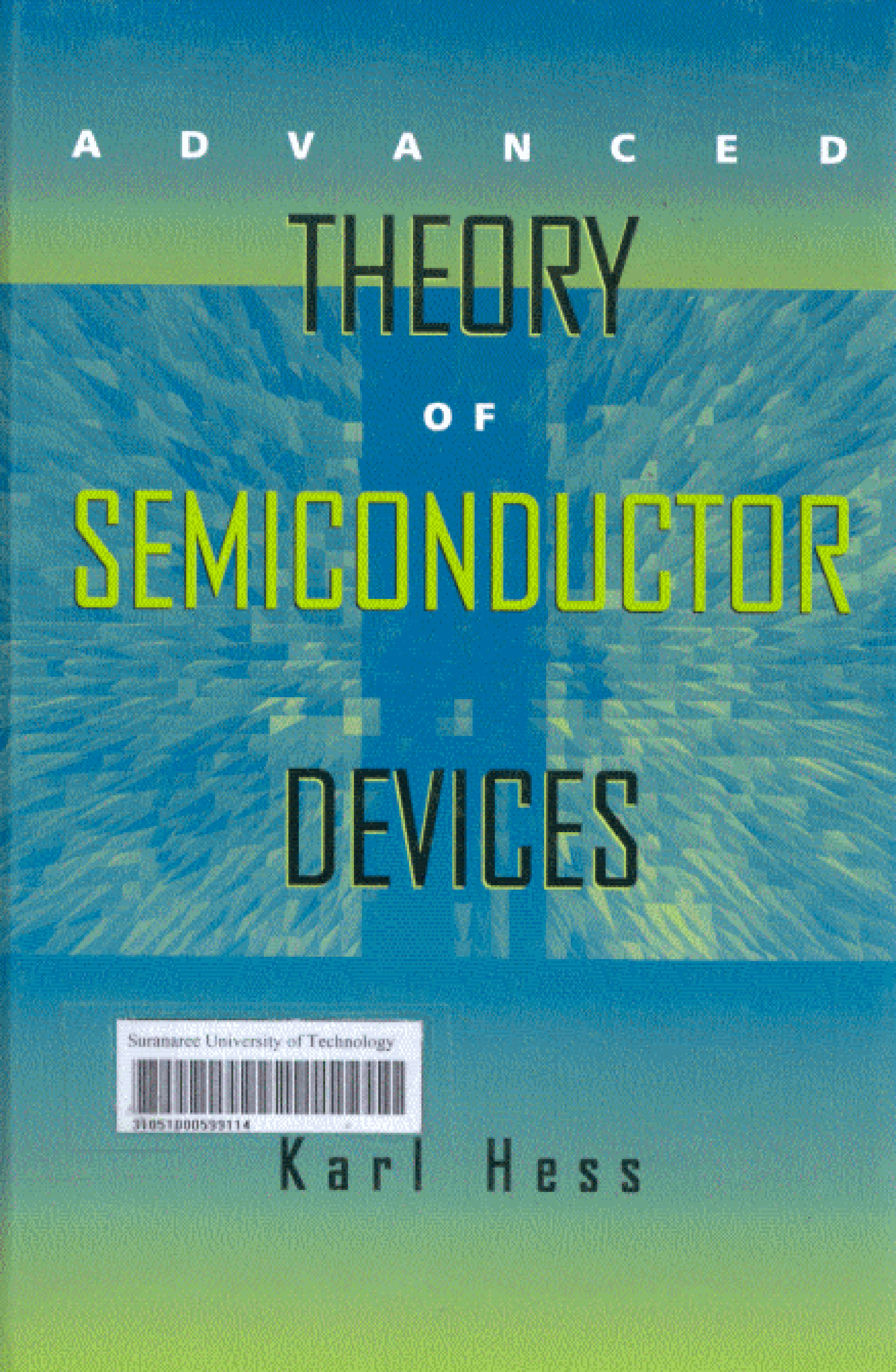

# ADVANCED THEORY OF SEMICONDUCTOR DEVICES

Karl Hess

# CONTENTS

**Preface** xiii

**Acknowledgments** xv

**Chapter 1 A Brief Review of the Basic Equations** 1
- 1.1 The Equations of Classical Mechanics, Application to Lattice Vibrations 2
- 1.2 The Equations of Quantum Mechanics 9

**Chapter 2 The Symmetry of the Crystal Lattice** 19
- 2.1 Crystal Structures of Silicon and GaAs 19
- 2.2 Elements of Group Theory 22
  - 2.2.1 Point Group 22
  - 2.2.2 Translational Invariance 26
- 2.3 Bragg Reflection 29

**Chapter 3 The Theory of Energy Bands in Crystals** 33
- 3.1 Coupling Atoms 33
- 3.2 Energy Bands by Fourier Analysis 34
- 3.3 Equations of Motion in a Crystal 42
- 3.4 Maxima of Energy Bands—Holes 46
- 3.5 Summary of Important Band-Structure Parameters 50
- 3.6 Band Structure of Alloys 50

**Chapter 4 Imperfections of Ideal Crystal Structure** 57
- 4.1 Shallow Impurity Levels—Dopants 58
- 4.2 Deep Impurity Levels 60
- 4.3 Dislocations, Surfaces, and Interfaces 62

**Chapter 5 Equilibrium Statistics for Electrons and Holes 67**

- 5.1 Density of States 67
- 5.2 Probability of Finding Electrons in a State 73
- 5.3 Electron Density in the Conduction Band 75

**Chapter 6 Self-Consistent Potentials and Dielectric Properties 81**

- 6.1 Screening and the Poisson Equation in One Dimension 82
- 6.2 Self-Consistent Potentials and the Dielectric Function 83

**Chapter 7 Scattering Theory 89**

- 7.1 General Considerations—Drude Theory 89
- 7.2 Scattering Probability from the Golden Rule 94
  - 7.2.1 Impurity Scattering 94
  - 7.2.2 Phonon Scattering 96
  - 7.2.3 Scattering by a δ-Shaped Potential 102
- 7.3 Important Scattering Mechanisms in Silicon and Gallium Arsenide 103

**Chapter 8 The Boltzmann Transport Equation 109**

- 8.1 Derivation 109
- 8.2 Solutions of the Boltzmann Equation in the Relaxation Time Approximation 114
- 8.3 Distribution Function and Current Density 121
- 8.4 Effect of Temperature Gradients and Gradients of the Band Gap Energy 125
- 8.5 Ballistic and Quantum Transport 127
- 8.6 The Monte Carlo Method 129

**Chapter 9 Generation-Recombination 135**

- 9.1 Important Matrix Elements 135
  - 9.1.1 Radiative Recombination 135
  - 9.1.2 Auger Recombination 139
- 9.2 Quasi-Fermi Levels (Imrefs) 139
- 9.3 Generation-Recombination Rates 140
- 9.4 Rate Equations 144

**Chapter 10 The Heterojunction Barrier 147**

- 10.1 Thermionic Emission of Electrons over Barriers 147

10.2 Free Carrier Depletion of Semiconductor Layers 151
10.3 Connection Rules for the Potential at an Interface 153
10.4 Solution of Poisson's Equation in the Presence of Free Charge Carriers 154
  10.4.1 Classical Case 154
  10.4.2 Quantum Mechanical Case 157
10.5 Pronounced Effects of Size Quantization and Heterolayer Boundaries 162

**Chapter 11 The Device Equations of Shockley and Stratton 167**
11.1 The Method of Moments 167
11.2 Moment for the Average Energy and Hot Electrons 170
  11.2.1 Steady-State Considerations 171
  11.2.2 Velocity Transients and Overshoot 175
  11.2.3 Equation of Poisson and Carrier Velocity 176

**Chapter 12 Numerical Device Simulations 181**
12.1 General Considerations 181
12.2 Numerical Solution of the Shockley Equations 184
  12.2.1 Numerical Simulation Beyond the Shockley Equations 188

**Chapter 13 Diodes 193**
13.1 Schottky Barriers—Ohmic Contacts 194
13.2 The *p–n* Junction 201
  13.2.1 Introduction and Basic Physics 201
  13.2.2 Basic Equations for the Diode Current 207
  13.2.3 Steady-State Current in Forward Bias 211
  13.2.4 AC Carrier Concentrations and Current in Forward Bias 213
  13.2.5 Short Diodes 215
  13.2.6 Recombination in Depletion Region 216
  13.2.7 Extreme Forward Bias 219
  13.2.8 Asymmetric Junctions 221
  13.2.9 Effects in Reverse Bias 223
13.3 High-Field Effects in Semiconductor Junctions 226
  13.3.1 Role of Built-In Fields in Electron Heating and *p–n* Junction Currents 226

- 13.3.2 Impact Ionization in $p$–$n$ Junctions 229
- 13.3.3 Zener Tunneling 236
- 13.3.4 Real Space Transfer 240

13.4 Negative Differential Resistance and Semiconductor Diodes 241

**Chapter 14 Laser Diodes 247**

14.1 Basic Geometry and Equations for Quantum Well Laser Diodes 248
14.2 Equations for Electronic Transport 250
14.3 Coupling of Carriers and Photons 253
14.4 Numerical Solutions of the Equations for Laser Diodes 257

**Chapter 15 Transistors 265**

15.1 Simple Models 266
- 15.1.1 Bipolar Transistors 266
- 15.1.2 Field Effect Transistors 272

15.2 Effects of Reduction in Size, Short Channels 278
- 15.2.1 Scaling Down Devices 278
- 15.2.2 Short Gates and Threshold Voltage 279

15.3 Hot Electron Effects 281
- 15.3.1 Mobility in Small MOSFETs 281
- 15.3.2 Impact Ionization, Hot Electron Degradation 284

**Chapter 16 Future Semiconductor Devices 291**

16.1 New Types of Devices 291
- 16.1.1 Extensions of Conventional Devices 291
- 16.1.2 Future Devices for Ultrahigh Integration 293

16.2 Challenges in Nanostructure Simulation 295
- 16.2.1 Nanostructures in Existing Semiconductor Devices 296
- 16.2.2 Quantum Dots 297
- 16.2.3 Structural, Atomistic, and Many-Body Effects 297

**Appendix A Tunneling and the Golden Rule 301**

**Appendix B The One Band Approximation 305**

Appendix C Temperature Dependence of the Band Structure 307

Appendix D Hall Effect and Magnetoresistance 309

Appendix E The Power Balance Equation 311

Appendix F The Self-Consistent Potential at a Heterojunction 315

Appendix G Schottky Barrier Transport 317

Index 321

About the Author 333