

High-speed heterostructure devices

From device concepts to circuit modeling

Fuelled by rapid growth in the communications industry, compound heterostructures and related high-speed semiconductor devices are spearheading the drive toward smaller, faster and lower-power electronics.

High-speed heterostructure devices is a textbook on modern high-speed semiconductor devices intended for both graduate students and practising engineers. This book is concerned with the underlying physics of heterostructures as well as practical analytical techniques for modeling and simulating these devices. Emphasis is placed on heterostructure devices of the present and of the immediate future such as the MODFET, HBT and RTD. The principles of operation of other devices such as the Bloch Oscillator, RITD, Gunn diode, quantum cascade laser and SOI and LD MOSFETs are also introduced.

Initially developed for a graduate course taught at The Ohio State University, the book comes with a complete set of homework problems and a web link to homework solutions and MATLAB programs supporting the lecture material.

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Patrick Roblin and Hans Rohdin
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To Gloria, Sébastien and Sophie
To the memory of Daga and Göte Rohdin

Contents

<i>Preface</i>	<i>page</i> xix
<i>Acknowledgements</i>	xxvi
<i>List of abbreviations</i>	xxix

Introduction	xxxi
---------------------	------

1	Heterostructure materials	1
1.1	Introduction	1
1.2	MBE technology	1
1.2.1	Lattice-matched systems	2
1.2.2	Pseudomorphic materials	3
1.2.3	The materials game and bandgap engineering	5
1.2.4	Limitations and applications of modern growth techniques	7
1.3	Crystal and reciprocal lattices	8
1.3.1	Crystals and lattices	8
1.3.2	The reciprocal lattice	9
1.3.3	Application to band structures	11
1.4	Conclusion	14
1.5	Bibliography	16
1.5.1	Recommended reading	16
1.5.2	References	16
1.6	Problems	16
2	Semiclassical theory of heterostructures	19
2.1	Introduction	19
2.2	Spatially-varying semiconductors	19
2.2.1	Semiconductor alloys	20

viii	Contents	
	2.2.2 Modulation doping	23
2.3	The Anderson band-diagram model	26
2.4	The abrupt heterojunction case	29
2.5	Drift-diffusion transport model for heterostructures	33
2.6	I – V characteristics of p–n heterojunctions	36
2.7	The thermionic model of heterojunctions	38
2.8	Ballistic launching	42
2.9	The HBT	44
2.10	Conclusion	46
	Appendix: Semiconductor parameter tables	46
2.11	Bibliography	46
	2.11.1 Recommended reading	46
	2.11.2 References	48
2.12	Problems	49
3	Quantum theory of heterostructures	53
3.1	Introduction	53
3.2	Band structures, Bloch functions and Wannier functions	54
	3.2.1 The Schrödinger equation	54
	3.2.2 Electron in a periodic potential	55
	3.2.3 Wannier functions	58
	3.2.4 Three-dimensional crystal	64
3.3	Spatially-varying band	68
	3.3.1 Heterojunction case (tight-binding approximation)	70
	3.3.2 Definition of the electron particle current (flux)	72
	3.3.3 Matching theory	76
	3.3.4 Three-dimensional effects	78
3.4	Multi-band tridiagonal Wannier picture	79
	3.4.1 Multi-band tridiagonal Wannier system	79
	3.4.2 Effective-mass wave-matching for a two-band Wannier system	81
	3.4.3 Comparison with a full-band model	84
3.5	Multi-band density of states	86
3.6	Conclusion	91
3.7	Bibliography	92
	3.7.1 Recommended reading	92
	3.7.2 References	92
3.8	Problems	93

ix	Contents	
4	Quantum heterostructure devices	97
4.1	Introduction	97
4.2	The accelerated band electron	98
4.2.1	Stark states and the Wannier ladder	98
4.2.2	Time-dependent solutions and the Houston state	102
4.2.3	The Bloch oscillator	104
4.2.4	Coherent and squeezed Zener oscillations	105
4.3	Quantum wells	106
4.3.1	Rectangular quantum wells	107
4.3.2	Quantum well induced by an electric field	108
4.3.3	Quantum wells of arbitrary shapes	109
4.3.4	Full-band structure effects	110
4.3.5	2DEG	110
4.4	Resonant tunneling	115
4.4.1	Double-barrier system	115
4.4.2	Tunneling current and resonant tunneling	119
4.4.3	Charge distribution inside the well	121
4.4.4	Exchange correlation	124
4.4.5	Scattering induced broadening	124
4.4.6	Full-band structure effects	124
4.4.7	High-frequency and high-speed response	128
4.4.8	Resonant interband tunneling diodes (RITDs)	128
4.5	Superlattice	129
4.5.1	Periodic superlattices	131
4.5.2	Random superlattice	133
4.5.3	Quasi-crystals and Fibonacci superlattices	135
4.6	Conclusion	137
4.7	Bibliography	138
4.7.1	Recommended reading	138
4.7.2	References	138
4.8	Problems	141
5	Scattering processes in heterostructures	148
5.1	Introduction	148
5.2	Phonons and phonon scattering	148
5.2.1	Phonons	152

x	Contents	
	5.2.2 Spontaneous and stimulated emissions	157
	5.2.3 Semiclassical phonon model	159
5.3	Polar scattering by optical phonons	161
5.4	Deformation potential scattering by acoustic phonons	162
5.5	Intervalley scattering by LO phonons	165
5.6	Interface roughness scattering	165
5.7	Alloy scattering	169
5.8	Electron–electron scattering	172
5.9	Conclusion	174
5.10	Bibliography	175
	5.10.1 Recommended reading	175
	5.10.2 References	175
5.11	Problems	176
6	Scattering-assisted tunneling	177
6.1	Introduction	177
6.2	Importance of three-dimensional scattering	178
6.3	Scattering-assisted tunneling theory	180
	6.3.1 Semiclassical scattering picture	180
	6.3.2 Matrix elements for the heterostructure Hamiltonian	181
	6.3.3 Matrix elements for the interaction Hamiltonian	181
	6.3.4 Envelope equations for sequential scattering	183
6.4	Transmission coefficient for scattering-assisted tunneling	186
6.5	Self-energy	188
6.6	The MSS algorithm	190
6.7	Scattering-parameter representation	194
6.8	Detailed balance and Pauli exclusion in MSS	198
6.9	Coupling functions for various scattering processes	204
6.10	Results for resonant tunneling structures	207
6.11	Conclusion	215
6.12	Bibliography	216
	6.12.1 Recommended reading	216
	6.12.2 References	216
6.13	Problems	217
7	Frequency response of quantum devices from DC to infrared	221
7.1	Introduction	221
7.2	Analytic solution for a uniform time-dependent potential	221

xi	Contents	
	7.3 Radiation coupling with an external modulated electric field	222
	7.4 Time-dependent tunneling theory	228
	7.5 Small-signal response without self-consistent potential	232
	7.6 Self-consistent solution	233
	7.7 RTD conductances and capacitances	237
	7.8 High-frequency response of the RTD	241
	7.9 Microwave measurement of the C – V characteristics	247
	7.10 DC bias instabilities	250
	7.11 Infrared response of quantum devices	251
	7.11.1 Modeling the infrared wave-guide	252
	7.11.2 Coupling of quantum transport with infrared radiation	254
	7.11.3 Optical absorption/emission coefficient	256
	7.11.4 Quantum cascade laser	259
	7.12 Conclusion	262
	7.13 Bibliography	263
8	Charge control of the two-dimensional electron gas	265
	8.1 Introduction	265
	8.2 2DEG population as a function of the Fermi energy	265
	8.3 Equilibrium population of the 2DEG	269
	8.4 Charge control of the 2DEG with a Schottky junction	272
	8.5 C – V characteristics of the MODFET capacitor	276
	8.6 I – V modeling of the Schottky junction	279
	8.7 Conclusion	282
	8.8 Bibliography	282
	8.9 Problems	283
9	High electric field transport	286
	9.1 Introduction	286
	9.2 The Boltzmann equation	287
	9.3 Electron transport in small electric fields	290
	9.3.1 Uniform semiconductor case	290
	9.3.2 Non-uniform semiconductor case	292
	9.4 Electron transport in a large electric field	294
	9.4.1 Uniform semiconductor case	294
	9.4.2 Non-uniform semiconductor case	296
	9.5 High-field transport: two-valley model	299
	9.6 Negative differential mobility and the Gunn effect	303

xii	Contents	
	9.7 Transient velocity overshoot in a time-varying field	308
	9.8 Stationary velocity overshoot in short devices	309
	9.9 Conclusion	310
	9.10 Bibliography	310
	9.10.1 Recommended reading	310
	9.10.2 References	310
	9.11 Problems	312
10	<i>I</i> – <i>V</i> model of the MODFET	314
	10.1 Introduction	314
	10.2 Long- and short-channel MODFETs	316
	10.3 Saturation and two-dimensional effects in FETs	323
	10.3.1 The Grebene–Ghandhi model	323
	10.3.2 Channel opening: MOSFET saturation model	331
	10.4 The extrinsic MODFET	337
	10.5 Conclusion	338
	10.6 Bibliography	338
	10.6.1 Recommended reading	338
	10.6.2 References	338
	10.7 Problems	339
11	Small- and large-signal AC models for the long-channel MODFET	342
	11.1 Introduction	342
	11.1.1 f_T and f_{max} figures of merit	342
	11.1.2 MAG and MSG	344
	11.1.3 Unilateral power gain of the wave-equation model	346
	11.1.4 On the ordering of f_T and f_{max}	347
	11.2 The MOSFET wave-equation (long-channel case)	350
	11.2.1 The large-signal MOSFET wave-equation	350
	11.2.2 Exact small-signal solution of the MOSFET wave-equation	351
	11.2.3 Frequency power series expansions of the y parameters	356
	11.2.4 Dimensionless representation of the y parameters	359
	11.2.5 First order equivalent circuit I	359
	11.2.6 Range of validity of the RC small-signal equivalent circuit I	361
	11.2.7 Alternative equivalent circuits for the intrinsic MODFET/MOSFET	363
	11.3 Large-signal model of the long-channel MODFET/MOSFET	365
	11.3.1 Charge conservation	373

xiii	Contents	
	11.3.2 Charge conservation in circuit simulators	374
	11.4 Parasitics, extrinsic MODFET and parameter extraction	376
	11.5 Conclusion	379
	11.6 Bibliography	379
	11.6.1 Recommended reading	379
	11.6.2 References	379
	11.7 Problems	381
12	Small- and large-signal AC models for the short-channel MODFET	384
	12.1 Introduction	384
	12.2 Small-signal model for the short-channel MOSFET	384
	12.2.1 The velocity-saturated MOSFET wave-equation	384
	12.2.2 Exact solution of the velocity-saturated MOSFET wave-equation	387
	12.2.3 Equivalent circuit of the velocity-saturated MOSFET wave-equation	389
	12.2.4 High-frequency performance of the short-channel MODFET	393
	12.2.5 Alternate equivalent circuit for the short-channel MODFET	395
	12.3 Large-signal model for the short-channel MOSFET	396
	12.3.1 First-order non-quasi-static approximation	397
	12.3.2 Small-signal equivalent circuit for the D'' internal node	400
	12.3.3 Large-signal model	403
	12.3.4 Charge-based representation	407
	12.3.5 Charge conservation	408
	12.3.6 Model topology	409
	12.4 Conclusion	410
	12.5 Bibliography	411
	12.6 Problems	411
13	DC and microwave electrothermal modeling of FETs	412
	13.1 Introduction	412
	13.2 Modeling for power amplifier design	413
	13.3 Physical versus table-based models	414
	13.4 Device characterization	415
	13.4.1 DC $I-V-T$	416
	13.4.2 Pulsed $I-V$ characteristics	416
	13.4.3 Isothermal $I-V$ characteristics	418
	13.5 Small-signal modeling	421
	13.5.1 Microwave data acquisition	421

xiv	Contents	
	13.5.2 Small-signal topology	421
	13.5.3 Parasitic deembedding	422
	13.6 Large-signal modeling	426
	13.6.1 Model formulation	426
	13.6.2 Tensor product B-splines	428
	13.6.3 I – V characteristics	430
	13.6.4 Parasitic bipolar topologies	431
	13.6.5 Charge	433
	13.7 Electrothermal modeling	433
	13.8 Circuit simulations	436
	13.8.1 Pulsed I – V characteristics	436
	13.8.2 Power amplifier	437
	13.9 Conclusion	439
	13.10 Bibliography	439
	13.11 Problems	441
14	Analytical DC analysis of short-gate MODFETs	442
	14.1 Introduction	442
	14.2 Background to the FET DC modeling approach	446
	14.3 Brief semiconductor materials history for SGBFETs	448
	14.4 2DEG gate charge control in a heavily dual pulse-doped MODFET structure	449
	14.5 An analytically manageable 2DEG transport model	458
	14.6 Quasi-two-dimensional model for electrostatics and I – V characteristics	460
	14.6.1 The low-field gradual channel	461
	14.6.2 Source, drain and contact resistances	464
	14.6.3 The high-field velocity-saturated region	466
	14.6.4 Impact ionization in the channel and gate tunneling	470
	14.6.5 Application examples and some large-signal issues	473
	14.7 Reliability	480
	14.8 Conclusion	482
	14.9 Bibliography	482
	14.10 Problems	489
15	Small-signal AC analysis of the short-gate velocity-saturated MODFET	490
	15.1 Introduction	490

xv	Contents	
	15.2 Equivalent circuit for the intrinsic device	490
	15.3 Displacement currents	498
	15.4 Conduction-induced currents and delays	507
	15.5 <i>Y</i> parameters and equivalent circuit for the extrinsic device	519
	15.6 Conclusion	524
	15.7 Bibliography	524
	15.8 Problems	525
16	Gate resistance and the Schottky-barrier interface	527
	16.1 Introduction	527
	16.2 Components in the input resistance	528
	16.3 Measurement and scaling of the gate resistance	530
	16.4 Interfacial gate resistance and Schottky barriers	534
	16.5 Admittance analysis of a Schottky barrier with semiconductor surface states	536
	16.6 Theory for the interfacial tunneling resistance	540
	16.6.1 General formalism for tunneling between metal and surface states	541
	16.6.2 Interfacial tunneling barrier	545
	16.6.3 Metal wave-function tail and tunneling effective mass	546
	16.6.4 Surface-state wave-function	548
	16.6.5 Tunneling resistance and capture cross-section	549
	16.7 Application to various Schottky-barrier models	550
	16.8 Summary and modifications to the equivalent circuit and <i>Y</i> -parameters	557
	16.9 Conclusion	562
	16.10 Bibliography	562
	16.11 Problems	565
17	MODFET high-frequency performance	567
	17.1 Introduction	567
	17.2 Some high-frequency measurement issues	567
	17.3 Recap of procedure and parameters for calculating MODFET <i>Y</i> parameters	572
	17.4 Current gain, optimum power gain and cut-off frequencies	576
	17.5 Optimization of f_{max}	580
	17.6 Noise, noise figure and associated gain	584
	17.6.1 The FET noise model by Pucel, Haus and Statz	589
	17.6.2 The Fukui equation and Pospieszalski's thermal model	591
	17.6.3 General formalism for noise figure and power gain	593

xvi	Contents	
	17.6.4 Noise figure and associated gain of the MODFET	595
	17.7 Process and manufacturability issues	600
	17.8 Reverse modeling	606
	17.9 Conclusion	607
	17.10 Bibliography	607
	17.11 Problems	611
18	Modeling high-performance HBTs	613
	18.1 Introduction	613
	18.2 Microscopic modeling of HBTs	614
	18.2.1 Introduction	614
	18.2.2 Direct solution of the BTE	614
	18.3 Compact modeling of HBTs	624
	18.3.1 Introduction	624
	18.3.2 Compact models for the collector current	624
	18.3.3 Compact models for f_T	632
	18.3.4 Compact models for f_{max}	641
	18.3.5 Compact model for large-signal analysis	643
	18.4 Conclusion	646
	18.5 Bibliography	647
	18.6 Problems	649
19	Practical high-frequency HBTs	651
	19.1 Introduction	651
	19.2 Material choices for HBTs	652
	19.2.1 History and evolution	652
	19.2.2 Growth techniques	656
	19.3 Processing techniques and device design	658
	19.3.1 Introduction	658
	19.3.2 III–V processing technology	658
	19.4 Further discussion of f_T , f_{max}	659
	19.4.1 Origin and distribution of delay times	659
	19.4.2 Improvement of delay times	661
	19.5 III–V surfaces and the emitter base saddle-point	665
	19.6 Thermal considerations	666
	19.7 Reliability issues	670
	19.7.1 Introduction	670

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Patrick Roblin and Hans Rohdin
Frontmatter
[More information](#)

xvii	Contents
	<hr/>
	19.7.2 The beryllium diffusion problem 670
	19.7.3 Beryllium diffusion solutions 673
	19.8 Conclusion 674
	19.9 Bibliography 675
	19.10 Problems 678
	<i>Index</i> 679

Preface

High-speed heterostructure devices is a textbook on modern high-speed semiconductor devices intended for both graduate students and practising engineers. This book is concerned with the physics and processes involved in the devices' operation as well as some of the most recent techniques for modeling and simulating these devices. Emphasis is placed on the heterostructure devices of the immediate future: namely the MODFET, HBT and RTD. The principle of operation of other devices such as the Bloch oscillator, RITD, Gunn diode, quantum cascade laser and SOI and LD MOSFETs is also introduced.

This text was initially developed for a graduate course taught at The Ohio State University and comes with a complete set of homework problems. MATLAB* programs are also available for supporting the lecture material. They can be used to regenerate a number of the pictures in the book and to assist the reader with some of the homework assignments.

This book should also prove useful to researchers and engineers, as it presents research material which is disseminated throughout the research literature and has never before been presented together in a book.

This text starts with two chapters reviewing the semiclassical theory of heterostructure devices. Five chapters are dedicated to presenting a realistic picture of heterostructures, introducing quantum devices and developing practical tools for analyzing quantum transport in these devices in the presence of scattering, and at high frequencies. One chapter is focused on the Boltzmann equation and its application to the derivation of moment equations for high-field transport. Five chapters are dedicated to reviewing the modeling of long- and short-channel FETs, including charge control, DC and high-frequency characteristics and the electrothermal modeling of FETs. This is followed by four chapters providing advanced DC and microwave modeling techniques, including a detailed analysis of parasitics in these devices. Finally the book concludes with two chapters dedicated to HBTs. A number of the chapters also provide practical design examples.

* MATLAB is a registered trademark of the MathWorks, Inc.

Required background

This text is intended for graduate students who have been introduced to semiconductor devices by a textbook of the level of Streetman’s *Solid State Electronic Devices*. A more advanced introduction to quantum mechanics, thermodynamics, band structure, phonons and devices is not assumed, as it is not realistic to request that the reader be familiar with all these theories. Our strategy is therefore to start from an undergraduate level and construct a more advanced theory of electronic heterostructure devices on this basis. However, there are a few concepts that we have not derived. The Boltzmann, Fermi–Dirac and Bose–Einstein distributions are postulated without a derivation from more fundamental principles. The results of the harmonic oscillator are also presented without a derivation. It is hoped that those graduate students not familiar with these topics will be motivated to take additional courses in classical thermodynamics, quantum theory, and semiconductor theory to enhance their understanding of those topics. But again this book is sufficiently self-contained that this is not a requirement.

Outline for the reader

Chapter 1 gives an overview of the device concepts introduced in all the chapters and motivates the need for these studies. This chapter also introduces MBE technology and its application to the growth of materials (alloys, pseudomorphic, modulation doped) for new device structures. The chapter concludes with a review of the cubic crystal structure and its reciprocal lattice.

Chapter 2 introduces the concept of heterostructures. Both gradually varying semiconductors (alloys) and abrupt heterojunctions are analyzed using the Anderson band-diagram model, and dipole correction effects are considered. The generalized low-field transport equations which apply to heterostructures are reviewed including the drift-diffusion and thermionic-diffusion models. A phenomenological model of ballistic electron launching is also presented. The principle of the heterojunction bipolar transistor is then introduced.

Chapter 3 presents a rigorous introduction to the concept of spatially-varying band structure using the generalized Wannier picture. Following a derivation of the Bloch theorem, the Wannier functions are introduced as the Fourier coefficients of the Bloch states and the Wannier recurrence equation is derived. For abrupt heterojunctions, the matrix elements of the heterojunction Hamiltonians are derived in the limit of the maximally transparent heterojunction. A multi-band density of states based on the impulse response is also introduced for the spatial identification of quantum resonances. The principal advantages of using the Wannier picture lie in: (1) its inherent capability to account rigorously for both the spatial variation of the band structure and its periodicity in \mathbf{k} space, and (2) its representation in terms of difference equations which are easily amenable to numerical solution.

Chapter 4 presents some fundamental one-dimensional quantum devices realizable using semiconductor heterostructures. The first class of devices discussed is that involving an accelerated electron in a band structure subjected to an applied electric field. Topics covered include the Wannier ladder and the Zener resonant tunneling effect, the Houston state and the acceleration theorem and finally wave-packets and squeezed states. The second class of devices considered is quantum wells. Topics covered include rectangular and triangular wells and the formation of a two-dimensional electron gas and subbands. The third class of devices considered is resonant tunneling and resonant interband tunneling diodes. Finally the fourth class of devices discussed focuses on superlattices, including the formation of minibands, wave-function localization in random superlattices and the fractal spectrum in Fibonacci superlattices.

Chapter 5 introduces the major scattering processes which limit the performance of quantum devices. Both elastic and inelastic scattering are considered. First the spectrum of lattice vibrations is presented and a semiclassical phonon model is introduced. The general form of the electron–phonon interaction Hamiltonian is then derived and the specific matrix elements for polar, acoustic, and intervalley phonon scattering processes evaluated. Next interface roughness scattering is analyzed using a model of uncorrelated terraces with a Gaussian distribution in size, and alloy scattering is analyzed using the virtual-crystal model. The chapter finishes with a discussion of electron–electron scattering.

Chapter 6 presents a realistic treatment of the impact of scattering upon tunneling-based devices using a direct three-dimensional ensemble-average solution of the Schrödinger equation. The importance of a three-dimensional analysis is first demonstrated. Next the scattering-assisted tunneling theory is shown to lead to a system of coupled Wannier recurrence equations enforcing current conservation. The formalism is then generalized to handle multiple sequential scattering processes and the Pauli exclusion effect with the introduction of the self-energy and the impulse response. Results for various resonant tunneling diodes (RTDs) are then presented for each scattering process, both individually and combined.

Chapter 7 studies tunneling in the presence of a time-varying interaction potential. The problem of an accelerated electron in a band subjected to both uniform DC and AC fields is solved exactly. A general rigorous analysis in terms of Fourier series is then given. The importance of self-consistently solving the Poisson and Schrödinger equations for calculating the current is demonstrated. Calculated small- and large-signal device impedances are presented for RTDs and an equivalent circuit is developed for their microwave simulation. The chapter concludes by studying how infrared radiation is coupled to ballistic quantum transport, and presents the principles of operation and recent results for the quantum cascade mid-infrared (10 μm) laser.

Chapter 8 covers the problem of the calculation of the 2DEG concentration in both gated and ungated MODFET capacitors. The self-consistent solution of the Schrödinger and Poisson equations is discussed, and an approximate analytic solution

based on the triangular well approximation is presented. The control of the 2DEG by a Schottky barrier, its high-frequency response and the MODFET capacitance are then modeled or analyzed. The chapter finishes with the modeling of the Schottky-barrier gate under forward bias.

Chapter 9 introduces simple transport models applicable to the MODFET and HBT. Transport in the electron gas is discussed using the Boltzmann equation. Approximate solutions are obtained for both small and large electric fields using the assumption of a drifted and heated Maxwell–Boltzmann distribution, and they are used to derive a generalized drift-diffusion current equation and its associated energy balance equation. These equations are solved to obtain the velocity–field relation in bulk silicon and GaAs, to analyze the Gunn effect, and to discuss transient and stationary overshoot in short-channel MOSFETs and MODFETs.

Chapter 10 is concerned with the I – V modeling of the MOSFET/MODFET. The I – V characteristic MOSFET/MODFET is studied using a simple charge control model and transport model. Emphasis is placed on studying short-channel effects and velocity saturation, and the threshold for their occurrence. A discussion of the two-dimensional field effects and their impact on the drain conductance is presented. For this analysis the Grebene–Ghandhi model, the channel opening model, and a full two-dimensional solution are compared.

Chapter 11 develops and solves the long-channel MOSFET/MODFET wave-equation. An optimal non-quasi-static equivalent circuit and a large-signal model approximating the large-signal MODFET wave-equations are then presented. The large-signal state equations are shown to conserve charge, and a charge-based representation suited for a circuit simulator is presented.

In Chapter 12 the velocity-saturated MODFET wave-equation is developed and solved for the short-channel MODFET. An optimal non-quasi-static equivalent circuit is presented and compared with the exact solutions. The long- and short-channel model topologies are also compared. Finally a charge-based large-signal model is presented for the short-channel MODFET.

Chapter 13 is concerned with the table-based electrothermal modeling of FETs for use in microwave circuit simulation. This chapter covers various topics such as device physics and model topology, measurement and characterization, parameter extraction and data presentation algorithms, and finally circuit design and simulation. The FET model topology introduced in Chapter 11 is augmented to account for the low-frequency dispersions associated with self-heating and the parasitic bipolar transistor. The need for and application of isothermal and pulsed DC and RF measurement techniques are reviewed. These concepts and modeling techniques are illustrated with examples from two major technologies: SOI for low-power RF CMOS and LDMOS for high-power linear amplification. However, the material presented is general enough that the techniques discussed can be applied to other devices.

Chapter 14 develops an accurate analytical model for the DC characteristics of MODFETs designed in industry for ultimate performance in high-speed communication and instrument applications. A thorough motivation for the approximate treatment is given. An overview of materials issues and evolution follows. The high doping and short gates used for these devices require a refined treatment of the charge control and transport, respectively. A quasi-two-dimensional model that includes mixed gate and drain charge control in regions internal and external to the gate is developed. I – V characteristics and the internal field distribution are obtained. These allow prediction of basic breakdown characteristics, which, in turn, affect the reliability of the devices, as is discussed.

Chapter 15 continues the analysis of cutting-edge MODFETs, but switches gear from DC to AC performance. The equivalent circuit is developed based on the theory in Chapter 11, and includes some important effects which occur in a velocity-saturated MODFET. These are studied with classical electrostatic approaches. In addition to standard capacitances, interesting effects are induced by transit delays in the device. The output conductance, a notoriously elusive parameter, is analyzed and predicted. The chapter concludes with an almost-complete extrinsic equivalent circuit. What is left for later is the inclusion of the distributed gate metalization resistance. First, an important topic that requires its own chapter has to be covered.

Chapter 16 focuses on an effect that requires a rather deep and different detour into semiconductor physics. The effect is the interfacial gate resistance which is of significant importance for device performance and scaling. In its purest form it is also of interest in the context of Schottky-barrier formation, a topic that has inspired a plethora of models, several of which are reviewed. Theories for dispersion and tunneling at the gate–semiconductor interface are developed. These require, in addition to familiar device and circuit analyses, a quantum mechanical treatment of a rather complex nature. Bardeen’s powerful view of tunneling is reviewed. The overlapping metal and semiconductor wave-functions are derived and motivated, respectively. The tunneling resistance is then derived. The various Schottky-barrier models can be accommodated by the model to produce theoretical values for the interfacial gate resistance. These are compared with the typical range of experimental values. After a summary and discussion of the results, the final extrinsic equivalent circuit for the velocity-saturated MODFET is arrived at.

After a brief overview of some high-frequency measurement issues, Chapter 17 uses the analytical physics-based MODFET equivalent circuit to predict and optimize the gain and noise. Two fundamental power gains and their cut-off frequencies are reviewed, as are three commonly used FET noise models. A general thermal noise model that accommodates the full extrinsic equivalent circuit is formulated and exercised. Some process and manufacturability issues affecting performance, yield, cost, and reliability are discussed. A very brief discussion on reverse modeling concludes this chapter on high-performance MODFETs.

Chapter 18 focuses on the modeling of the heterojunction bipolar transistor (HBT). Compact models for HBTs are developed with the intention of providing tractable equations for predicting the DC, small-signal AC, and large-signal properties of high-frequency and high-power devices. The models are connected to fundamental theory by appealing to results from a microscopic theory of transport based on a direct solution of the Boltzmann transport equation.

Chapter 19, our last chapter, gives the reader an in-depth look at examples of the device physics issues that must be faced in realizing the HBT devices described theoretically in Chapter 18. It covers the application of arsenide and phosphide compound semiconductor material systems to HBTs in detail. The main device-design problems for high-speed HBTs, and their interaction with fabrication, are described. An example of the problems posed by practical III–V surfaces is provided by an examination of the emitter–base saddle-point effect in AlGaAs/GaAs HBTs. The effect of material choice on the important area of thermal properties is described. Finally, this chapter examines long-term device degradation, using beryllium diffusion as an example to study the defect chemistry behind the problem.

Recommendations for the instructor

This book is best suited for a semester course. By focusing on device concepts rather than mathematical derivations during the lecture it is possible to cover one chapter a week. The mastery of the mathematical techniques presented is then acquired by the students when they complete the homework problems. These homework problems indeed usually motivate a careful reading of the derivations presented in each chapter.

New graduate students are generally sufficiently prepared by conventional undergraduate textbooks/courses to take this graduate course. An exception, however, is the concept of Brillouin zone and \mathbf{k} space which is not often well mastered if it has been covered at all. To address this problem a review of the cubic crystal structure and its reciprocal lattice is included in Chapter 1. The concept of \mathbf{k} space is also heuristically introduced in Chapter 1 before being rigorously derived in Section 3.2.2 for one dimension and in Section 3.2.4 for three dimensions using the translation operator.

We have found it to be of critical importance to provide the students with simple MATLAB* programs implementing the techniques presented. These MATLAB* programs serve multiple purposes. First they allow many of the figures in the text to be regenerated. The students can then vary the parameters and do simple experiments. Sometimes these tools are also used in exercises to verify the validity of analytic calculations. This is particularly important for the quantum calculations which can be quite abstract until the students start reproducing the results themselves. This literally

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brings this material to life. A special web site is available from Cambridge University Press or from <http://eewww.eng.ohio-state.edu/~roblin/cupbook> for downloading these MATLAB[†] programs. We will keep adding new problems and programs to support this text. A correction set for most of the homework problems can also be downloaded by instructors from the same web site.

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Acknowledgements by Patrick Roblin

The writing of a graduate textbook on *high-speed heterostructure devices* has been a project that I conceived early in my research and teaching career with the motivation of presenting fundamental device concepts as well as addressing challenging modeling issues faced by researchers and engineers in this field. The realization of such a book would not have been possible, however, without the help of many researchers, and I would like to acknowledge them here. First, this book is the result of the cooperative writing of many experts in their fields. My coauthor contributed four key chapters on the state-of-the-art design and modeling of MODFETs, in addition to contributing an insightful and critical review of the overall manuscript. My PhD student, Dr Siraj Akhtar, now at Texas Instruments, cowrote with me a chapter on electrothermal modeling of FETs. Finally we invited two experts in HBT to contribute to this book. Prof. David Pulfrey of the University of British Columbia contributed a chapter on the modeling of high-frequency HBTs, and Dr Nick Moll of Agilent Laboratories contributed a chapter on the practical and theoretical know-how required for building high-performance HBTs.

The chapters that I contributed are for the most part based on original research papers published in the literature or on research conducted with my MS and PhD students at OSU. Therefore I would like in particular to thank my PhD students, Dr Young Min Kim, Dr Sung Choon Kang, Prof. Wan Rone Liou, Dr Chih Ju Hung and Dr Siraj Akhtar for their key contributions. My group was also enhanced by the important contributions of several postdoctoral researchers, Dr Paul Sotirelis, the late Prof. Gene Cao, and Dr Dae Kwan Kim. The contributions of many of these researchers would not have been possible without the research funding support provided by US government agencies (NSF and NEMO project) and US industry, principally Cray, Allied Signal, Texas Instruments and Lucent Technologies.

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xxviii Acknowledgements

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Columbus	P. R.
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	July 2001

List of abbreviations

1SS	single-sequential scattering
2DEG	two-dimensional electron gas
2DHG	two-dimensional hole gas
3DEG	three-dimensional electron gas
AMPS	advanced mobile phone service
AUDM	advanced unified defect model
bcc	body-centered cubic
BJT	bipolar junction transistor
BTE	Boltzmann transport equation
CAD	computer-aided design
CDMA	code division multiple access
DBS	direct broadcast satellite
DDE	drift-diffusion equation
DHBT	double-heterojunction bipolar transistor
DIGS	disorder-induced gap state
DUT	device under test
FATFET	long-gate FET
fcc	face-centered cubic
FDMA	frequency division multiple access
FET	field-effect transistor
GCA	gradual-channel approximation
HBT	heterojunction bipolar transistor
HEMT	high-electron-mobility transistor
HFET	heterostructure field-effect transistor
HTOL	high-temperature operating lifetime
IC	integrated circuit
IF	intermediate frequency
JWKB	Jeffreys–Wentzel–Kramers–Brillouin
LGLTB	linearly-graded low-temperature buffer
LNA	low-noise amplifier
LRM	line, reflect, match
MBE	molecular beam epitaxy

xxx **List of abbreviations**

MESFET	metal–semiconductor field-effect transistor
MIGS	metal-induced gap state
MISFET	metal–insulator–semiconductor field-effect transistor
MMIC	monolithic microwave integrated circuits
MOCVD	metal organic chemical vapor deposition
MODFET	modulation-doped field-effect transistor
MSS	multiple-sequential scattering
MSSCAT	multiple-sequential scattering-assisted tunneling
MTTF	mean time to failure
NDC	negative differential conductivity
NDR	negative differential resistivity
NEGF	non-equilibrium Green’s function
NWA	network analyzer
OEIC	optoelectronic integral circuits
OMVPE	organometallic vapor phase epitaxy
PA	power amplifier
PAE	power-added efficiency
PDC	positive differential conductivity
PE	Poisson’s equation
PECVD	plasma-enhanced chemical vapor deposition
PHEMT	pseudomorphic high-electron-mobility transistor
PHS	Pucel, Haus and Statz
POP	polar-optical phonon
RF	radio frequency
RFOL	RF operating lifetime
RIE	reactive ion etch
RITD	resonant interband tunneling diode
RTD	resonant tunneling diode
SBGFET	Schottky-barrier-gate field-effect transistor
SDHT	selectively doped heterojunction transistor
SEM	scanning electron microscopy
SHBT	single-heterojunction bipolar transistor
SII	screened ionized impurity
SOI	silicon on insulator
SOLT	short, open, load, thru
SPICE	simulation program for integrated circuit emphasis
SWE	Schrödinger wave-equation
TEGFET	two-dimensional electron gas field-effect transistor
TPS	tensor product spline
VCO	voltage controlled oscillator
WKB	Wentzel–Kramers–Brillouin

Introduction

It is the trend in the silicon and compound microelectronic technology to continuously develop semiconductor circuits which are faster, smaller, and consume less power for a similar level of integration. This has been recently fueled in part by the rapid growth of digital wireless communication, which relies on both low-power high-speed digital and high-frequency analog electronics. As part of this trend, microwave, RF and IF analog and digital circuits are being integrated in ‘mixed-signal’ circuits for wireless applications. Both silicon and compound state-of-the-art integrated circuits presently rely on high-speed state-of-the-art submicron devices. However, research in microelectronic technology is always expanding its frontier; new heterostructure semiconductor materials and devices are continuously being developed or improved in a process often referred to as bandgap engineering. These heterostructure devices, in particular, and high-speed devices, in general, constitute the subject of this book. In this book we take the readers on a journey providing them with an understanding of both fundamental and advanced device-physics concepts as well as introducing them to the development of realistic device models which can be used for the design, simulation and modeling of high-speed electronics.

The journey in this book takes the reader from the fundamental physical processes taking place in heterostructures to the practical issues involved in designing high-performance heterostructure devices.

Ever shrinking high-speed devices

It is a basic requirement that high-speed devices must be small. Reducing the device reduces the transit-time and the capacitances in devices. The operating voltage is also reduced, and this helps with the reduction of the power dissipation. There are a few exceptions, i.e., devices which do not rely on the transit-time principle, but essentially this principle holds so far for the field-effect and bipolar transistors which are the engine of today’s microelectronics. The shrinking of the device is occurring both horizontally, as defined by lithography, and vertically, as defined by growth and processing techniques. For example MOSFETs and MODFETs of 0.085 μm or 850 Å

gate length are becoming very common. Even more striking are the modern growth techniques which have made possible the vertical growth of new semiconductor devices with unprecedented control. One of the most versatile growth techniques available for research is molecular beam epitaxy (MBE) which permits one to deposit one atomic layer at a time while abruptly or gradually changing the semiconductor material and doping type. The capability of MBE growth techniques will be reviewed in Chapter 1.

Quantum effects

In Chapter 2 we will explore the semiclassical modeling of heterostructures by reviewing how the bulk and junction theory has been extended to deal with them. However, as the device size keeps shrinking, quantum effects clearly become important and must be considered. This occurs when the device dimension compares with the mean free path of the electrons. In fact many fundamental questions are raised when dealing with very small devices. Traditionally semiconductors are theoretically introduced as crystals which are by definition periodic structures repeating indefinitely. But how can a band structure now be rigorously defined in spatially-varying semiconductors? To address this question we will introduce in Chapter 3 a special quantum picture, the generalized Wannier representation, which will describe the formation of the bands at the lattice level. In fact we shall see that it takes typically about ten lattice parameters for the band structure to be well defined away from an interface or surface. The generalized Wannier representation will also permit us to discuss in Chapter 4 transport problems such as the Bloch oscillations which have long both fascinated and challenged device physicists.

Quantum devices

Quantum devices are devices which directly exploit quantum effects. Various types of quantum devices have been conceived, including quantum wells, superlattices and resonant tunneling diodes (RTDs). Superlattices are periodic heterostructures forming a synthesized one-dimensional crystal. Superlattices can be used, for example, to generate the elusive Bloch oscillations. The study of random superlattices will permit us to gain insight into the conductor–insulator transition which takes place when the superlattice periodicity is destroyed.

With a couple of periods of a superlattice we can form a double-barrier potential system, which is transparent to electrons when the barrier separation corresponds to a multiple of half their wavelength. This effect is the basis for the RTD which exhibits a negative differential up to terahertz. The RTD, which is the fastest active

semiconductor diode available so far, is a very important test device, as it is based on a quantum effect and yet operates at room temperature. It also finds applications in high-speed digital and microwave circuits.

Finally, one of the key quantum effects we shall study is the creation of a two-dimensional electron gas (2DEG) by quantum confinement. The 2DEG is of particular importance as it is used as the channel of the fastest FET developed: the MODFET. Chapter 8 will therefore be dedicated to studying how we can control this 2DEG with a gate voltage at both DC and high frequency.

From quantum transport to Boltzmann equation

To the first order, transport in quantum devices is typically ballistic. That is the electrons travel with out being scattered. However, even in quantum devices the ballistic transport approximation is not realistic, and scattering processes must be accounted for. How do we solve the Schrödinger equation in the presence of phase-breaking scattering processes? We shall address this subject in Chapter 6 and develop a realistic theory bridging the gap between the ideal ballistic transport model and the semiclassical Boltzmann transport theory. As we shall see, the electron wave-functions are effectively attenuated in their propagation as they spawn new scattered waves through various possible scattering processes. The exploitation of quantum effects in quantum devices is therefore only possible when the spatial variation device structure is smaller than the mean free path. Indeed, it is only when the electron wave-function has a well-defined phase that interferences, which are a requirement of quantum wave effects, can effectively take place.

Ballistic transport versus drift-diffusion transport

Even when quantum effects are negligible we will find it necessary to identify whether or not ballistic transport or/and drift-diffusion is taking place. These are indeed the two fundamentally different regimes of transport which can both take place, sometimes simultaneously, inside a device.

Consider the simple pastoral scene of a lake with a waterfall on one side and a small creek on the other. There is clearly a continuous flow of water from the waterfall, through the lake and into the creek. However, if the lake is very wide, the water drift might not even be perceptible to a fisherman on its bank fishing for trout. But a fly-fisherman fishing in the creek will see his dry fly quickly drift away and will need to recast his line often. If a red dye or some kind of liquid trout food is poured into the lake at one spot we expect it to slowly diffuse and spread throughout the lake. A drift-diffusion model therefore applies well to the lake area. On the other hand, no