

# Contents

<b>1</b>	<b>Introduction</b> .....	1
	Hassan Raza	
1.1	Overview .....	1
1.2	Book Summary .....	7
1.3	Outlook .....	10
	References .....	11

## Part I Metrology and Synthesis

<b>2</b>	<b>Raman Spectroscopy: Characterization of Edges, Defects, and the Fermi Energy of Graphene and <math>sp^2</math> Carbons</b> .....	15
	M.S. Dresselhaus, A. Jorio, L.G. Cançado, G. Dresselhaus, and R. Saito	
2.1	Introduction to the Resonance Raman Spectra of Graphene .....	15
2.1.1	The Raman Spectra of $sp^2$ Carbons .....	16
2.1.2	Edge Structure of Graphene .....	18
2.1.3	The Multiple-Resonance Raman Scattering Process ...	18
2.1.4	Concept of the Kohn Anomaly .....	21
2.1.5	Introduction to Near-Field Raman Spectroscopy .....	22
2.2	Characterization of Defects .....	22
2.2.1	Point Defects Induced by Ion Bombardment .....	23
2.2.2	Model for the D-Band Activated Region .....	24
2.2.3	Line Defects at the Edges of Nanographene .....	26
2.3	Characterization of Edges .....	29
2.3.1	Overview of Graphene Edges .....	29
2.3.2	The Characterization of Graphene Edges from Their <i>D</i> -Band Scattering .....	30
2.3.3	Mode assignments of the Raman Spectra of Graphene Nanoribbons .....	34
2.3.4	Polarization Dependence of the Raman Intensity .....	38

2.4	The Fermi Energy Dependence: The Kohn Anomaly .....	40
2.4.1	Effect of Gate Doping on the <i>G</i> -Band of Single-Layer Graphene .....	40
2.4.2	Effect of Gate Doping on the <i>G</i> Band of Double-Layer Graphene .....	42
2.5	Near-Field Raman Spectroscopy .....	44
2.5.1	The Spatial Resolution in Optical Microscopes .....	45
2.5.2	The Principle of TERS .....	45
2.5.3	Mechanism of Near-Field Enhancement.....	46
2.5.4	Application to Carbon Nanotubes.....	47
2.6	Summary and Perspective .....	49
	References.....	53
<b>3</b>	<b>Scanning Tunneling Microscopy and Spectroscopy of Graphene .....</b>	<b>57</b>
	Guohong Li and Eva Y. Andrei	
3.1	Introduction .....	57
3.2	STM/STS Techniques .....	58
3.3	Sample Preparation .....	61
3.4	Hallmarks of Graphene in STM/STS .....	61
3.5	Line Shape of Landau Levels .....	66
3.6	Electron–phonon Coupling .....	67
3.7	Coupling Between Graphene Layers.....	69
3.8	Twist Between Graphene Layers.....	71
3.8.1	Appearance of Moiré Pattern.....	72
3.8.2	Saddle Point Van Hove Singularities.....	73
3.8.3	Single Layer-like Behavior and Velocity Renormalization .....	73
3.9	Graphene on SiO <sub>2</sub> .....	77
3.9.1	Three Types of Corrugations .....	77
3.9.2	Scanning Tunneling Spectroscopy .....	79
3.9.3	Quantum Interference and Fermi Velocity.....	79
3.9.4	Trapped Charges in SiO <sub>2</sub> .....	80
3.10	Edges, Defects and Magnetism.....	81
3.11	SPM-based Nano-lithography .....	82
3.11.1	Signs of Invasiveness of an STM Tip .....	83
3.11.2	Folding Graphene Layers.....	83
3.11.3	Cutting Graphene Layers .....	84
3.11.4	Surface Modification .....	85
3.12	Summary and Perspectives .....	87
	References.....	88
<b>4</b>	<b>The Electronic Properties of Adsorbates on Graphene .....</b>	<b>93</b>
	Eli Rotenberg	
4.1	Introduction: What Are Adsorbates on Graphene Good for?.....	93
4.2	Angle-Resolved Photoemission Spectroscopy .....	96
4.2.1	Introduction .....	96

4.2.2	Band Structure Determination of Graphene .....	96
4.2.3	Self-energy Determination .....	99
4.3	The “Zoology” of Adsorbates .....	102
4.3.1	Adsorption of Nontransition-Metal Atoms .....	103
4.3.2	Adsorption of Transition Metal Atoms .....	107
4.4	Adsorbate–Graphene Interactions: General Symmetry Considerations .....	110
4.5	Hydrogen on Graphene As a Prototype Adsorbate System .....	112
4.5.1	Introduction .....	112
4.5.2	Hydrogen on Graphene: Experimental Evidence for Anderson Localization .....	114
4.6	Potassium on Graphene: The Coulomb Interaction in Graphene, Revealed .....	118
4.6.1	K Adsorption on Epitaxial Graphene on SiC(0001) ...	118
4.6.2	K Adsorption on Quasi-free-Standing Epitaxial Graphene on SiC(0001) .....	120
4.7	Calcium Adsorption: Superconducting Instability of Graphene .....	124
4.8	Conclusions and Outlook .....	128
	References .....	129
<b>5</b>	<b>Epitaxial Graphene on SiC(0001)</b> .....	<b>135</b>
	Thomas Seyller	
5.1	Introduction .....	135
5.2	Silicon Carbide and Its Polar Surfaces .....	137
5.3	Growth of Epitaxial Graphene on SiC(0001) in Ultra-High Vacuum .....	138
5.4	The $(6\sqrt{3} \times 6\sqrt{3})R30^\circ$ Reconstruction .....	140
5.5	Electronic Structure of Monolayer and Bilayer Graphene at the K-point .....	143
5.6	State-of-the Art Graphene Growth in Argon Atmosphere .....	146
5.7	Transport Properties of Graphene on SiC(0001) .....	149
5.8	Engineering the Interface Between Graphene and SiC(0001) by Hydrogen Intercalation .....	152
5.9	Conclusion .....	155
	References .....	155
<b>6</b>	<b>Magneto-Transport on Epitaxial Graphene</b> .....	<b>161</b>
	Peide D. Ye, Michael Capano, Tian Shen, Yanqing Wu, and Michael L. Bolen	
6.1	Introduction .....	161
6.2	Epitaxial Graphene Synthesis .....	163
6.3	Dielectric Integration on Epitaxial Graphene .....	168
6.4	Top-Gate Graphene Field-Effect Transistors .....	169
6.5	Half-Integer Quantum Hall-Effect in Epitaxial Graphene .....	172
6.6	Ballistic and Coherent Transport on Epitaxial Graphene .....	178

6.7	Spin Transport on Epitaxial Graphene .....	183
6.8	Summary .....	185
	References .....	185
<b>7</b>	<b>Epitaxial Graphene on Metals .....</b>	<b>189</b>
	Yuriy Dedkov, Karsten Horn, Alexei Preobrajenski, and Mikhail Fonin	
7.1	Introduction .....	189
7.2	Methods of Graphene Preparation on Metal Surfaces.....	193
7.3	Experimental Methods.....	194
7.4	Graphene on Lattice-Matched $3d$ -Metal Surfaces .....	197
	7.4.1 Atomic Structure of Graphene Layer on Ni(111) and Co(0001).....	198
	7.4.2 Electronic Structure of Graphene on Lattice-Matched Surfaces .....	200
	7.4.3 Magnetism of Graphene on the Ni(111) Surface .....	206
7.5	Graphene on Lattice-Mismatched $4d$ , $5d$ -Metal Surfaces.....	209
	7.5.1 Structure of Graphene on Ir(111), Ru(0001), and Rh(111) .....	210
	7.5.2 Electronic Structure of Graphene on Lattice-Mismatched Surfaces .....	214
7.6	Hybrid Structures on the Basis of Graphene Layers on Metal Surfaces .....	218
	7.6.1 Intercalation-like Systems .....	219
	7.6.2 Growth of Noble Metal Clusters on Graphene Moirè .....	222
	7.6.3 Growth of Magnetic Metal Clusters on Graphene Moirè .....	225
	7.6.4 Chemical Functionalization of Graphene on Transition Metal Surfaces .....	226
7.7	Conclusions and Outlook .....	228
	References .....	230

## Part II Electronic-structure and Transport Properties

<b>8</b>	<b>Electronic Properties of Monolayer and Bilayer Graphene .....</b>	<b>237</b>
	Edward McCann	
8.1	Introduction .....	237
8.2	The Crystal Structure of Monolayer Graphene .....	238
	8.2.1 The Real Space Structure.....	238
	8.2.2 The Reciprocal Lattice of Graphene .....	239
	8.2.3 The Atomic Orbitals of Graphene.....	239
8.3	The Tight-Binding Model .....	240
8.4	The Tight-Binding Model of Monolayer Graphene .....	242
	8.4.1 Diagonal Matrix Elements.....	242
	8.4.2 Off-Diagonal Matrix Elements .....	244

8.4.3	The Low-Energy Electronic Bands of Monolayer Graphene .....	246
8.5	Massless Chiral Quasiparticles in Monolayer Graphene.....	248
8.5.1	The Dirac-Like Hamiltonian .....	248
8.5.2	Pseudospin and Chirality in Graphene.....	249
8.6	The Tight-Binding Model of Bilayer Graphene .....	251
8.7	Massive Chiral Quasiparticles in Bilayer Graphene.....	254
8.7.1	The Low-Energy Bands of Bilayer Graphene .....	254
8.7.2	The Two-Component Hamiltonian of Bilayer Graphene .....	255
8.7.3	Pseudospin and Chirality in Bilayer Graphene .....	256
8.8	The Integer Quantum Hall Effect in Graphene .....	258
8.8.1	The Landau Level Spectrum of Monolayer Graphene .....	258
8.8.2	The Integer Quantum Hall Effect in Monolayer Graphene .....	260
8.8.3	The Landau Level Spectrum of Bilayer Graphene .....	261
8.8.4	The Integer Quantum Hall Effect in Bilayer Graphene .....	262
8.9	Trigonal Warping in Graphene .....	263
8.9.1	Trigonal Warping in Monolayer Graphene .....	263
8.9.2	Trigonal Warping and Lifshitz Transition in Bilayer Graphene .....	264
8.10	Tuneable Band Gap in Bilayer Graphene .....	266
8.10.1	Asymmetry Gap in the Band Structure of Bilayer Graphene .....	266
8.10.2	Self-Consistent Model of Screening in Bilayer Graphene .....	268
8.11	Summary .....	272
	References.....	273
<b>9</b>	<b>Electronic Properties of Graphene Nanoribbons .....</b>	<b>277</b>
	Katsunori Wakabayashi	
9.1	Introduction .....	277
9.2	Electronic States of Graphene .....	279
9.2.1	Tight-Binding Model and Edge States .....	281
9.2.2	Massless Dirac Equation .....	284
9.2.3	Edge Boundary Condition and Intervalley Scattering .....	286
9.3	Electronic Transport Properties .....	287
9.3.1	One-Way Excess Channel System .....	288
9.3.2	Model of Impurity Potential.....	291
9.3.3	Perfectly Conducting Channel: Absence of Anderson Localization .....	291

9.4	Universality Class .....	293
9.4.1	Graphene Nanoribbons with Generic Edge Structures .....	294
9.5	Transport Properties Through Graphene Nanojunction .....	296
9.6	Summary .....	297
	References .....	298
<b>10</b>	<b>Mesoscopics in Graphene: Dirac Points in Periodic Geometries .....</b>	<b>301</b>
	H.A. Fertig and L. Brey	
10.1	Graphene Ribbons .....	303
10.1.1	Hamiltonian .....	303
10.1.2	Zigzag Nanoribbons .....	304
10.1.3	Armchair Nanoribbons .....	307
10.2	Graphene Quantum Rings .....	310
10.2.1	Chirality in Armchair Nanoribbons .....	311
10.2.2	Phase Jumps at Corner Junctions .....	312
10.2.3	Numerical Results .....	314
10.3	Graphene in a Periodic Potential .....	317
10.3.1	Counting Dirac Points .....	317
10.3.2	Numerical Solutions of the Dirac Equation .....	320
10.3.3	Conductivity .....	320
10.4	Conclusion .....	322
	References .....	322
<b>11</b>	<b>Electronic Properties of Multilayer Graphene .....</b>	<b>325</b>
	Hongki Min	
11.1	Introduction .....	325
11.1.1	Stacking Arrangements .....	326
11.1.2	$\pi$ -Orbital Continuum Model .....	327
11.2	Energy Band Structure .....	327
11.2.1	Preliminaries .....	327
11.2.2	Monolayer Graphene .....	328
11.2.3	AA Stacking .....	329
11.2.4	AB Stacking .....	331
11.2.5	ABC Stacking .....	333
11.2.6	Arbitrary Stacking .....	334
11.3	Landau-Level Spectrum .....	336
11.3.1	Preliminaries .....	336
11.3.2	AA Stacking .....	336
11.3.3	AB Stacking .....	337
11.3.4	ABC Stacking .....	339
11.3.5	Arbitrary Stacking .....	339
11.4	Low-Energy Effective Theory .....	341
11.4.1	Introduction .....	341
11.4.2	Pseudospin Hamiltonian .....	341

11.4.3	Stacking Diagrams .....	342
11.4.4	Partitioning Rules .....	342
11.4.5	Degenerate State Perturbation Theory .....	344
11.4.6	Limitations of the Minimal Model .....	347
11.4.7	Effects of the Consecutive Stacking .....	347
11.5	Applications .....	348
11.5.1	Quantum Hall Conductivity .....	348
11.5.2	Optical Conductivity .....	350
11.5.3	Electrical Conductivity .....	351
11.6	Conclusions .....	354
	References .....	355
<b>12</b>	<b>Graphene Carrier Transport Theory .....</b>	<b>357</b>
	Shaffique Adam	
12.1	Introduction .....	357
12.2	Graphene Boltzmann Transport .....	360
12.2.1	Screening: Random Phase Approximation (RPA).....	362
12.2.2	Coulomb Scatterers .....	365
12.2.3	Gaussian White Noise Disorder .....	366
12.2.4	Yukawa Potential .....	367
12.2.5	Gaussian Correlated Impurities .....	367
12.2.6	Midgap States .....	368
12.3	Transport at Low Carrier Density .....	369
12.3.1	Self-Consistent Approximation .....	371
12.3.2	Effective Medium Theory .....	377
12.3.3	Magneto-Transport and Temperature Dependence of the Minimum Conductivity .....	381
12.3.4	Quantum to Classical Crossover .....	383
12.3.5	Summary of Theoretical Predictions for Coulomb Impurities.....	386
12.4	Comparison with Experiments .....	387
12.4.1	Magnetotransport: Dependence of $\sigma_{xx}$ and $\sigma_{xy}$ on Carrier Density .....	387
12.4.2	Dependence of $\sigma_{\min}$ and Mobility on Impurity Concentration .....	389
12.4.3	Dependence of $\sigma_{\min}$ and Mobility on Dielectric Environment .....	389
12.5	Conclusion .....	391
	References .....	392
<b>13</b>	<b>Exploring Quantum Transport in Graphene Ribbons with Lattice Defects and Adsorbates .....</b>	<b>395</b>
	George Kirczenow and Siarhei Ihnatsenka	
13.1	Landauer Theory of Transport .....	397
13.2	Subband Structure and Transport in Ideal Ribbons .....	399
13.3	Quantized Ballistic Conductance.....	402

13.4	Electron Transport in Graphene Ribbons .....	403
13.5	Discovery of Quantized Conductance in Strongly Disordered Graphene Ribbons .....	404
13.6	The Roles of Different Classes of Defects .....	405
13.7	Tight Binding Model of Ribbons with Edge Disorder, Interior Vacancies, and Long-Ranged Potentials .....	406
13.8	Numerical Simulations of Quantum Transport .....	406
13.8.1	Disorder-Induced Conductance Suppression, Fluctuations and Destruction of the Ballistic Quantized Conductance Plateaus .....	408
13.8.2	Conductance Dips at the Edges of Ribbon Subbands .....	410
13.8.3	The Role of Temperature .....	411
13.8.4	From Ballistic Transport to Anderson Localization ....	412
13.8.5	The Quantized Conductance in Disordered Ribbons: Theory vs. Experiment .....	414
13.9	Adsorbates on Graphene and Dirac Point Resonances .....	416
13.9.1	Tight Binding Hamiltonian for Adsorbates on Graphene .....	417
13.9.2	Effective Hamiltonian for Adsorbates on Graphene ...	419
13.9.3	The T-matrix Formalism .....	420
13.9.4	Dirac Point Scattering Resonances due to H, F, and O Atoms and OH Molecules Adsorbed on Graphene .....	421
13.10	Electron Quantum Transport in Graphene Ribbons with Adsorbates .....	423
13.10.1	Building Efficient Tight-Binding Models .....	423
13.10.2	Results of Numerical Simulations of Quantum Transport in Ribbons with Adsorbates .....	426
13.11	Summary .....	431
	References .....	431
<b>14</b>	<b>Graphene Oxide: Synthesis, Characterization, Electronic Structure, and Applications .....</b>	<b>435</b>
	Derek A. Stewart and K. Andre Mkhoyan	
14.1	Introduction .....	436
14.2	Understanding Bulk Graphite Oxide and Graphene Oxide Monolayers .....	437
14.3	Fabrication of Graphite Oxide and Graphene Oxide .....	439
14.3.1	Traditional Approaches to Fabricate Graphite Oxide .....	440
14.3.2	New Fabrication Techniques for Graphite Oxide and Graphene Oxide .....	441



14.4	Characterization Approaches .....	444
14.4.1	Optical Microscopy .....	444
14.4.2	Scanning Transmission Electron Microscopy .....	445
14.4.3	Electron Energy Loss Spectroscopy .....	447
14.4.4	Atomic Force Microscopy .....	448
14.4.5	X-ray Photoelectron Spectroscopy .....	449
14.4.6	Raman Spectroscopy of Graphene Oxide and Reduced Graphene .....	451
14.5	Insight from Simulations .....	452
14.5.1	Using Epoxy Groups to Unzip Graphene .....	452
14.5.2	Graphene Oxide Electronic Structure .....	454
14.5.3	Electron Mobility and Transport .....	455
14.6	Applications for Graphene Oxide .....	457
14.6.1	Graphene Oxide Electronics.....	457
14.6.2	Sensors .....	458
14.6.3	Carbon-Based Magnetism .....	458
14.7	Future Perspectives .....	459
	References.....	460

**Part III From Physics and Chemistry of Graphene to Device Applications**

<b>15</b>	<b>Graphene <i>pn</i> Junction: Electronic Transport and Devices .....</b>	<b>467</b>
	Tony Low	
15.1	Introduction .....	467
15.2	Transport in the Absence of a Magnetic Field.....	469
15.2.1	Dirac Equation, Pseudospin, and Chirality .....	470
15.2.2	Abrupt <i>pn</i> Junction and Analogy with Optics .....	472
15.2.3	Tunneling for Dirac and Schrödinger Fermions .....	474
15.2.4	Quantum Transport Modeling .....	477
15.2.5	Experiments: Asymmetry and odd Resistances .....	479
15.3	Transport in the Presence of Magnetic Fields .....	482
15.3.1	Weak Magnetic Field Regime .....	482
15.3.2	Edge States, Snake States, and Valley Isospin.....	485
15.3.3	Quantum Hall Regime: The Ballistic Case .....	487
15.3.4	Experiments: Ballistic to Ohmic Transition .....	490
15.4	Transport in the Presence of Strain-Induced Pseudo-Magnetic Fields .....	494
15.4.1	Strain-Induced Pseudo-Magnetic Field .....	494
15.4.2	Edge States and Transport Gap.....	497
15.4.3	Magnetic and Electric Snake States .....	501
15.5	Discussions .....	503
15.5.1	Devices: Current Status and Outlook .....	503
15.5.2	Conclusions .....	505
	References.....	505

<b>16</b>	<b>Electronic Structure of Bilayer Graphene Nanoribbon and Its Device Application: A Computational Study</b> .....	509
	Kai-Tak Lam and Gengchiao Liang	
16.1	Introduction .....	509
16.2	Methodology .....	511
16.3	Electronic Structure of Monolayer Graphene Nanoribbon.....	512
16.3.1	Armchair Edges .....	512
16.3.2	Zigzag Edges .....	513
16.3.3	Dopant Effect .....	514
16.4	Electronic Structure of Bilayer Graphene Nanoribbon.....	516
16.4.1	Armchair Edges .....	517
16.4.2	Zigzag Edges with Dopants .....	518
16.4.3	Interlayer Distance .....	518
16.5	Bilayer Graphene Nanoribbon Device .....	519
16.6	Bilayer ZGNR NEM Switch .....	521
16.7	Conclusion .....	524
	References.....	525
<b>17</b>	<b>Field-Modulation Devices in Graphene Nanostructures</b> .....	529
	Hassan Raza	
17.1	Introduction .....	529
17.2	Electronic Structure .....	530
17.3	Theoretical Framework: Extended Hückel Theory .....	533
17.4	Bilayer Graphene .....	535
17.4.1	<i>A–B</i> stacking .....	536
17.4.2	Strain Engineering .....	536
17.4.3	Misalignment .....	538
17.5	Armchair Graphene Nanoribbons .....	538
17.5.1	Pristine Edges .....	539
17.5.2	Periodic edge roughness effects .....	543
17.6	Zigzag Graphene Nanoribbons with Periodic Edge Roughness .....	546
17.7	Novel Applications .....	550
17.8	Conclusions .....	551
	References.....	552
<b>18</b>	<b>Graphene Nanoribbons: From Chemistry to Circuits</b> .....	555
	F. Tseng, D. Unluer, M.R. Stan, and A.W. Ghosh	
18.1	The Innermost Circle: The Atomistic View .....	556
18.1.1	Flatland: A Romance in Two Dimensions .....	557
18.1.2	Whither Metallicity? .....	558
18.1.3	Edge Chemistry: Benzene or Graphene? .....	559
18.1.4	Whither Chirality? .....	561
18.2	The Next Circle: Two Terminal Mobilities and <i>I–Vs</i> .....	563
18.2.1	Current–Voltage Characteristics ( <i>I–Vs</i> ).....	563

18.2.2	Low Bias Mobility-Bandgap Tradeoffs: Asymptotic Band Constraints .....	566
18.3	The Third Level: Active Three-Terminal Electronics .....	569
18.3.1	Wide–Narrow–Wide: All Graphene Devices .....	569
18.3.2	Solving Quantum Transport and Electrostatic Equations .....	570
18.3.3	Improved Electrostatics in 2-D .....	571
18.3.4	Three-Terminal I–Vs .....	574
18.3.5	Pinning vs. Quasi-Ohmic Contacts .....	575
18.4	The Penultimate Circle: GNR Circuits.....	576
18.4.1	Geometry of An All Graphene Circuit.....	577
18.4.2	Compact Model Equations .....	579
18.4.3	Digital Circuits.....	579
18.4.4	How ‘Good’ is a Graphene-based Invertor? .....	580
18.4.5	Physical Domain Issues: Monolithic Device-Interconnect Structures .....	583
18.5	Conclusions .....	583
	References.....	585
	<b>Index</b> .....	587



<http://www.springer.com/978-3-642-20467-8>

Graphene Nanoelectronics

Metrology, Synthesis, Properties and Applications

Raza, H. (Ed.)

2012, XXIII, 598 p. 277 illus., 202 illus. in color.,

Hardcover

ISBN: 978-3-642-20467-8