

Contents

1 Carbon Materials	1
1.1 History	1
1.2 Hybridization in A Carbon Atom	4
1.2.1 sp Hybridization: Acetylene, $\text{HC}\equiv\text{CH}$	5
1.2.2 sp^2 Hybridization: Polyacetylene, $(\text{HC}=\text{CH}-)_n$	7
1.2.3 sp^3 Hybridization: Methane, (CH_4)	8
1.2.4 Carbon $1s$ Core Orbitals	9
1.2.5 Isomers of Carbon	11
1.2.6 Carbynes	13
1.2.7 Vapor Grown Fibers	14
2 Tight Binding Calculation of Molecules and Solids	17
2.1 Tight Binding Method for a Crystalline Solid	17
2.1.1 Secular Equation	17
2.1.2 Procedure for obtaining the energy dispersion	21
2.2 Electronic Structure of Polyacetylene	22
2.3 Two-Dimensional Graphite	25
2.3.1 π Bands of Two-Dimensional Graphite	26
2.3.2 σ Bands of Two-Dimensional Graphite	29
3 Structure of a Single-Wall Carbon Nanotube	35
3.1 Classification of carbon nanotubes	35
3.2 Chiral Vector: C_h	37
3.3 Translational Vector: T	39
3.4 Symmetry Vector: R	41
3.5 Unit Cells and Brillouin Zones	45
3.6 Group Theory of Carbon Nanotubes	48
3.7 Experimental evidence for nanotube structure	53

4	Electronic Structure of Single-Wall Nanotubes	59
4.1	One-electron dispersion relations	59
4.1.1	Zone-Folding of Energy Dispersion Relations	59
4.1.2	Energy Dispersion of Armchair and Zigzag Nanotubes	61
4.1.3	Dispersion of chiral nanotubes	65
4.2	Density of States, Energy gap	66
4.3	Effects of Peierls distortion and nanotube curvature	70
5	Synthesis of Carbon Nanotubes	73
5.1	Single-Wall Nanotube Synthesis	73
5.2	Laser Vaporization Synthesis Method	74
5.3	Arc Method of Synthesizing Carbon Nanotubes	77
5.4	Vapor Growth and Other Synthesis Methods	79
5.4.1	Vapor Growth Method	80
5.4.2	Other Synthesis Methods	82
5.5	Purification	83
5.6	Nanotube Opening, Wetting, Filling and Alignment	84
5.6.1	Nanotube Opening	84
5.6.2	Nanotube Wetting	85
5.6.3	Nanotube Filling	85
5.6.4	Alignment of Nanotubes	86
5.7	Nanotube Doping, Intercalation, and BN/C Composites	86
5.8	Temperature Regimes for Carbonization and Graphitization	87
5.9	Growth Mechanisms	89
6	Landau Energy Bands of Carbon Nanotubes	95
6.1	Free Electron in a Magnetic Field	95
6.2	Tight Binding in a Magnetic Field	98
6.3	Cosine Band in a Magnetic Field	100
6.4	Landau Energy Bands	104
6.5	Landau Energy Bands: Aharonov-Bohm	108
6.6	Landau Energy Bands: Quantum-Oscillation	111
7	Connecting Carbon Nanotubes	115
7.1	Net Diagrams of a Junction	115
7.2	The Rule for Connecting Two Nanotubes	119

7.3	Shape of a Junction	120
7.4	Tunneling Conductance of a Junction	123
7.5	Coiled Carbon Nanotubes	130

8	Transport Properties of Carbon Nanotubes	137
8.1	Quantum transport in a one-dimensional wire	137
8.1.1	A ballistic conductor ($L \ll L_m, L_\varphi$)	142
8.1.2	Classic transport, $L_\varphi \ll L_m \ll L$	144
8.1.3	Localization, ($L_m \ll L_\varphi \ll L$)	145
8.1.4	Universal Conductance Fluctuations	148
8.1.5	Negative Magnetoresistance	151
8.2	Transport experiments on carbon nanotubes	152
8.2.1	Attaching Contacts	153
8.2.2	An Individual Single-Wall Nanotube	154
8.2.3	An Individual Rope of Single-Wall Nanotubes	158
8.2.4	Magneto-Transport in Multi-Wall Nanotubes	159

9	Phonon Modes of Carbon Nanotubes	163
9.1	Dynamical matrix for phonon dispersion relations	163
9.2	Phonon dispersion relations for two-dimensional graphite	165
9.3	Phonon dispersion relations for nanotubes	171
9.3.1	Zone folding method	171
9.3.2	Force constant tensor of a carbon nanotube	173
9.3.3	Force constant corrections due to curvature of 1D nanotubes	178

10	Raman Spectra of Carbon Nanotubes	183
10.1	Raman or infrared active modes of carbon nanotubes	183
10.2	Raman experiments on single-wall nanotubes	187
10.3	Bond Polarizability Theory of Raman Intensity for Carbon Nanotubes	192
10.4	Raman Spectra of Nanotubes with Random Orientations	195
10.4.1	Lower Frequency Raman Spectra	196
10.4.2	Higher Frequency Raman Modes	198
10.4.3	Medium Frequency Raman Modes	201
10.5	Sample Orientation Dependence	203

11 Elastic Properties of Carbon Nanotubes	207
11.1 Overview of Elastic Properties of Carbon Nanotubes	207
11.2 Strain Energy of Carbon Nanotubes	210
11.3 The Peierls Instability of Nanotubes	213
11.3.1 Bond Alternation	213
11.3.2 Peierls Distortion of graphite and carbon nanotubes . . .	217
11.4 Properties of Multi-Wall Nanotubes	221
References	239
Index	253