



Hiroyuki Shima
Motohiro Sato

Elastic and Plastic Deformation of Carbon Nanotubes



Hiroyuki Shima
Motohiro Sato

Elastic and Plastic Deformation of Carbon Nanotubes

Contents

<i>Preface</i>	xiii
1 Introduction	1
1.1 Carbon Nanotube: The World's Stiffest Material	1
1.2 Discovery before 1991: Who Found It First?	4
1.2.1 Matter in Issue	4
1.2.2 Historical Facts	5
1.2.3 Closing Remark	7
2 Young's Modulus Measurement	9
2.1 Introduction	9
2.2 Thermally Induced Vibration	10
2.3 Electrically Induced Vibration	12
2.4 Singly Clamped Deflection	13
2.5 Doubly Clamped Deflection	15
2.6 Tensile Loading	19
3 Atomistic Modeling	21
3.1 Introduction	21
3.2 Methodology	22
3.2.1 <i>Ab initio</i> Method	22
3.2.2 Tight-Binding Method	23
3.2.3 Molecular Dynamics Method	24
3.3 Comparison: Quantum or Classical?	24
3.4 Interatomic Potential	25
3.4.1 Tersoff and First-Generation Brenner Potential	25
3.4.2 Second-Generation Brenner Potential	27
3.5 Young's Modulus Prediction	29
3.6 Via <i>ab initio</i> Approach	31

3.7	Via Tight-Binding Approach	33
3.8	Via MD Approach	34
3.8.1	Dependence on Diameter and Chirality	37
4	Continuum Modeling	39
4.1	Introduction	39
4.2	Young's Modulus	40
4.3	Axial Rigidity for Bars and Trusses	42
4.4	Bending Rigidity for Beams	43
4.5	Axial and Bending Rigidity for Shells	45
4.6	Young's Modulus Prediction	46
4.6.1	C-C Bond Modeling Using Truss and Beam Elements	46
4.6.2	Modeling Using Beams and Shells	48
4.6.3	Bridging Atomistic and Continuum Modeling	52
4.7	Cauchy-Born Rule	53
4.8	Multishell Nanotube Elasticity	56
4.9	Crystal of SWNTs	56
5	Buckling	59
5.1	Better Bend than Break	59
5.2	Resilience and Sensitivity	61
5.3	Bend Buckling of SWNTs	62
5.3.1	Kink Formation	62
5.3.2	Diameter Dependence	64
5.3.3	Transient Bending	65
5.4	Bend Buckling of MWNTs	67
5.4.1	Ripples Emerging	67
5.4.2	Yoshimura Pattern	68
5.5	Twist Buckling	71
5.5.1	Asymmetric Response	71
5.5.2	Non-Trivial Responses	73
5.6	Universal Non-Linear Scaling	75
5.7	Radial Corrugation under Pressure	77
6	Topological Defects	81
6.1	Defects in Carbon Nanotubes	81
6.2	Stone-Wales Transformation	82

6.3	Formation Energy	84
6.4	Strain-Induced Defect	86
6.4.1	Atomistic View	86
6.4.2	Energetics	88
6.5	Direct Micrograph Image	90
6.6	Curvature Generation	91
6.7	Fusion of Adjacent Nanotubes	96
7	Fracture	99
7.1	Failure Strength	99
7.2	Tensile Load Measurements	100
7.3	Discrepancy Resolved	101
7.4	One-Atom Vacancy Effect	102
7.5	Large-Hole Effect	104
8	Super-Elongation	107
8.1	Candy-Making of a Nanotube	107
8.2	Bond Flip Mechanism	108
8.3	From Brittle to Ductile	111
8.4	Interdependence in the Failure Mechanism	114
8.5	C ₂ Removal Mechanism	116
8.6	Mono-Atomic C-Chain	118
9	Carbon Nanocoil	121
9.1	Merits of Coiled Structures	121
9.2	Synthesis of Carbon Nanocoils	123
9.3	Microscopic Model of Carbon Nanocoils	124
9.4	Spring Constant of Carbon Nanocoils	126
9.5	Superelasticity of Carbon Nanocoils	127
9.6	Coil Geometry Statistics	129
9.7	Cushioning Effect	131
10	Irradiation-Based Tailoring	135
10.1	What Can Be Done by Irradiation?	135
10.2	High-Energetic Particles Workable	137
10.3	Self-Healing of Vacancies	138
10.3.1	Overview	138
10.3.2	Microscopic view	140

10.4	Relax from a One-Atom Vacancy	142
10.4.1	In Armchair SWNT	142
10.4.2	In Zigzag SWNT	144
10.5	Radial Shrinkage of SWNTs	145
10.6	Internal Collapse of MWNTs	147
10.7	Inner-Wall Corrugation by Outer-Wall Erosion	149
10.8	Exhibition of Various Tailoring Techniques	151
10.8.1	Fusion of Adjacent SWNTs	151
10.8.2	Cutting and Bending	153
10.8.3	Welding into Branched Nanotubes	154
11	Internal Sliding	157
11.1	Potential Nano-“Trombone”	157
11.2	Low-Friction Sliding	159
11.2.1	Initial Theoretical Prediction	159
11.2.2	Experimental Observation	160
11.2.3	Gigahertz Oscillator Inspired	162
11.3	Shell-by-Shell Extraction	163
11.4	Internal Rotation	165
11.5	Telescopic Oscillation	167
11.5.1	Mechanism	167
11.5.2	Oscillation Frequency Estimation	168
11.5.3	Perspective	170
11.6	Plucking a Nano-“Guitar” String	171
12	Unzipping	175
12.1	Toward Graphene Nanoribbon Production	175
12.2	Acid Reaction Method	178
12.3	Plasma Etching	179
12.4	Intercalation-Induced Exfoliation	180
12.5	Catalytic Cutting	182
12.6	Current-Induced Breakdown	183
13	Reinforcement Application	187
13.1	As the Ultimate Reinforced Fibers	187
13.2	Critical Challenges: Adhesion, Dispersion, Alignment	188
13.3	Mixture Rules and Beyond	190

13.3.1	Mixture Rule: Long-Fiber Situation	190
13.3.2	Shear-Lag Model: Short-Fiber Situation	192
13.4	Reinforcement by Millimeter-Long Nanotubes	194
13.5	Critical Length for Fiber Breaking	196
13.6	Interfacial Coupling Strength	197
13.6.1	Breakthrough Wanted	197
13.6.2	Category of Interfacial Couplings	199
13.7	Pullout Test	201
13.8	Polymer Reinforcement	203
13.8.1	Solution Process	203
13.8.2	Melting Process	203
13.8.3	Thermosetting Process	204
13.8.4	Functionalization Process	205
13.9	Ceramics and Metal Reinforcement	207
	<i>Bibliography</i>	209
	<i>Index</i>	251