

# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
<b>2</b>	<b>Methodology of Quantum Mechanics/Atomic Simulations</b>	<b>5</b>
2.1	Method for Electronic Structure Calculation	5
2.1.1	Fundamental Approximations for Electronic Structure Calculation	6
2.1.2	Hartree–Fock Method	6
2.1.3	Density-functional Theory	8
2.2	First-Principles Calculation with Plane Wave Basis Set	9
2.2.1	Kohn–Sham Equation	9
2.2.2	Local Density Approximation	10
2.2.3	Generalized Gradient Approximation	13
2.2.4	Pseudopotential Method and Norm-Conserving Pseudopotential	14
2.2.5	Hamiltonian in NCPP	15
2.2.6	Ultrasoft Pseudopotential Method	18
2.2.7	Projector-augmented Wave Method	20
2.2.8	All-Electron Method	22
2.2.9	Beyond LDA and GGA	23
2.2.10	Evaluation of Physical Quantities	24
2.3	Semi-empirical and Empirical Theories for Nanostructure Properties	28
2.3.1	Semi-empirical Calculation of Electronic State	28
2.3.2	Atomistic Modeling Using Empirical Interatomic Potential	31
2.4	Conclusion	32
	References	33

<b>3</b>	<b>Ideal Strength in Low-Dimensional Nanostructures</b>	35
3.1	Mechanical Properties of Nanostructures	35
3.1.1	Ideal Strength	35
3.1.2	Elastic Constants	39
3.2	Ideal Understructure	40
3.2.1	Zero-Dimensional Understructure	40
3.2.2	One-Dimensional Understructure	41
3.2.3	Two-Dimensional Understructure	43
3.2.4	Understructure of Two or More Elements	44
3.3	Nanostructures with Ideal Shape	45
3.3.1	Two-Dimensional Nanostructures	46
3.3.2	One-Dimensional Nanostructures	56
3.3.3	Zero-Dimensional Nanostructures	63
3.4	Conclusion	64
	References	65
<b>4</b>	<b>Strain Engineering on Nanosemiconductors</b>	67
4.1	Strain Engineering on Semiconductors	67
4.2	Bulk Semiconductors	68
4.2.1	Bulk Semiconductors Subjected to External Strain	68
4.2.2	Bulk Semiconductors with Internal Strain Fields	71
4.3	Nanosemiconductors	74
4.3.1	Two-Dimensional Nanosemiconductors	74
4.3.2	One-Dimensional Nanosemiconductors	80
4.3.3	Zero-Dimensional Nanosemiconductors	90
4.4	Conclusion	94
	References	94
<b>5</b>	<b>Ferroelectric Nanostructures</b>	97
5.1	Ferroelectricity in Bulk	97
5.1.1	Ferroelectric Instability and Its Response to Strain	97
5.1.2	Domain Structure and Domain Switching	98
5.1.3	Effect of Defects	102
5.2	Thin Film and Surface Property: Two-Dimensional Structure	103
5.2.1	Ferroelectric Surface Structure	103
5.2.2	Correlation Between Surface Structure and Internal Geometry	108
5.2.3	Ferroelectric Thin-Film Capacitor	114
5.3	Nanowire and Nanotube: One-Dimensional Structure	120
5.3.1	FE Structure in Perovskite Nanowire	120
5.3.2	FE Perovskite Nanotube	124
5.3.3	Strain Effect in Nanowire and Nanotube	128

5.4	Nanodot: Zero-Dimensional Structure. . . . .	134
5.5	Conclusion . . . . .	137
	References. . . . .	137
<b>6</b>	<b>Magnetism in Nanostructures. . . . .</b>	<b>141</b>
6.1	Magnetism in Bulk. . . . .	141
6.1.1	Magnetism and Its Response to Strain. . . . .	141
6.2	Thin Film and Monolayer: Two-Dimensional Structure . . . . .	146
6.2.1	Thin Films and Surface Properties. . . . .	146
6.2.2	Monolayer. . . . .	149
6.3	Nanowire, Nanotube, and Atomic Chain: One-Dimensional Structure. . . . .	154
6.3.1	Nanowires . . . . .	154
6.3.2	Nanotubes . . . . .	155
6.3.3	Atomic Chains. . . . .	159
6.4	Atomic Cluster: Zero-Dimensional Structure . . . . .	162
6.5	Conclusion . . . . .	163
	References. . . . .	163
<b>7</b>	<b>Multiferroic Nanostructures . . . . .</b>	<b>165</b>
7.1	Multiferroicity in Bulk . . . . .	165
7.1.1	Multiferroic Properties and Response to Strain . . . . .	165
7.1.2	Multiferroic Domains and Domain Walls . . . . .	167
7.1.3	Atomic Defects . . . . .	169
7.2	Multiferroicity in Nanostructures . . . . .	172
7.2.1	Nanofilms and Surface Properties: Two-Dimensional Structure . . . . .	172
7.2.2	Nanowires: One-Dimensional Structure. . . . .	177
7.3	Extrinsic (Defect-Induced) Multiferroics in Atomic Scales. . . . .	181
7.3.1	Multiferroic Grain Boundaries with Oxygen Vacancies . . . . .	182
7.3.2	Multiferroic Vacancies at Ferroelectric Oxide Surfaces . . . . .	185
7.3.3	Strain-Induced Multiferroic Transitions . . . . .	188
7.4	Conclusion . . . . .	190
	References. . . . .	190
<b>8</b>	<b>Ferroic Nanometamaterials and Composites . . . . .</b>	<b>193</b>
8.1	Ferroic Nanometamaterials from Phase-Field Modeling . . . . .	193
8.1.1	Phase-Field Modeling of Ferroelectrics . . . . .	194
8.1.2	Phase-field Modeling of Ferromagnetic Systems . . . . .	196
8.1.3	Phase-field Modeling of Multiferroic Composites . . . . .	199

8.2	Nanometamaterials of Ferroelectrics . . . . .	201
8.2.1	Unusual Domain Patterning in Nanometamaterials . . . . .	201
8.2.2	Tunable Polar and Toroidal Electromechanical Properties . . . . .	204
8.2.3	Multiple Hysteresis Behaviors . . . . .	206
8.3	Multiferroic Nanocomposites . . . . .	210
8.4	Conclusion . . . . .	212
	References. . . . .	213

Multiphysics in Nanostructures

Umeno, Y.; Shimada, T.; Kinoshita, Y.; Kitamura, T.

2017, X, 214 p. 116 illus., 91 illus. in color., Hardcover

ISBN: 978-4-431-56571-0