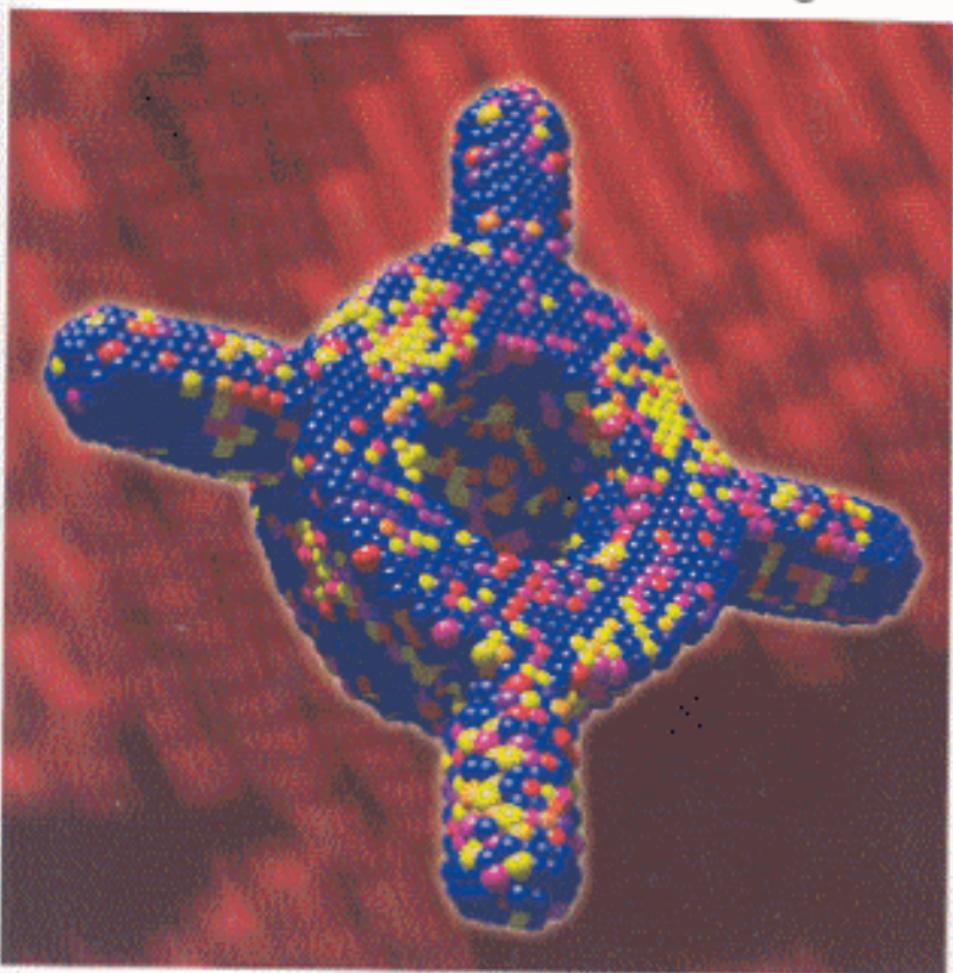


Series on the Foundations of Natural Science and Technology – Vol. 6

Michael Rieth

Nano-Engineering in Science and Technology

An Introduction to the World of Nano-Design



World Scientific

Contents

Preface	v
Chapter 1 Introduction	1
Chapter 2 Interatomic Potentials	7
2.1 Quantum Mechanical Treatment of the Many-Particle Problem	7
2.2 Potential Energy Surface	10
2.3 Pair Potential Approximation	12
2.4 Advantages and Limitations of the Pair Potential Approximation	13
2.5 Phenomenological Potentials	15
2.5.1 Buckingham Potentials	16
2.5.2 Morse Potentials	17
2.5.3 Lennard-Jones Potentials	18
2.5.4 Barker Potentials for Krypton and Xenon	20
2.6 Pseudo Potentials	22
2.6.1 Schommers Potential for Aluminium	27
2.7 Many-Body Potentials	29
Chapter 3 Molecular Dynamics	33
3.1 Models for Molecular Dynamics Calculations	35
3.1.1 Initial Values	36
3.1.2 Isothermal Equilibration	41
3.1.3 Boundaries	43
3.1.4 Nano-Design and Nano-Construction	46

3.2	Visualization Techniques	48
3.3	Solution of the Equations of Motion	51
3.3.1	Verlet Algorithms	53
3.3.2	Nordsieck/Gear Predictor-Corrector	54
3.3.3	Assessment of the Integration Algorithms	57
3.3.4	Other Methods	58
3.3.5	Normalized Quantities	58
3.4	Efficient Force Field Computation	59
3.4.1	Force Derivation	59
3.4.2	List Method	60
3.4.3	Cell Algorithms	61
3.4.4	SPSM Procedure	62
3.4.5	Discussion	64
3.5	Implementation	65
Chapter 4 Characterization of Nano-Systems		67
4.1	Thermal Stability	67
4.2	Basic Material Properties	70
4.3	Wear at the Nanometer Level	75
4.4	Mean Values and Correlation Functions	75
4.4.1	Ensemble Theory	77
4.4.2	Pair Correlation Function	79
4.4.3	Mean-Square Displacement	81
4.4.4	Velocity Auto-Correlation Function	83
4.4.5	Generalized Phonon Density of States	85
4.4.6	Structure Factor	87
4.4.7	Additional Remarks	90
Chapter 5 Nano-Engineering — Studies and Conclusions		91
5.1	Functional Nanostructures	92
5.2	Nano-Machines	96
5.3	Nano-Clusters	102
5.3.1	Structural Examinations	103
5.3.2	Dynamics of the Al ₅₀₀ States	108
5.3.3	Influence of the Initial Conditions	110
5.3.4	Influence of the Initial Temperature	112
5.3.5	Influence of the Crystalline Structure	112
5.3.6	Influence of the Outer Shape and Cluster Size	113
5.3.7	Influence of the Interaction Potential (Material)	119

Contents

xi

5.3.8 Conclusions	120
5.4 Stimulated Nano-Cluster Transformations	122
5.5 Analogy Considerations	125
5.6 The Bifurcation Phenomenon at the Nanometer Scale	127
5.7 Analogies to Biology	128
5.8 Final Considerations	129
Bibliography	133
Index	139