

Contents

Preface *xiii*

1	Classical Theory and Atomistics	1
1.1	Law of Friction	1
1.2	The Origin of Friction	4
1.3	Atomistics in Tribology	6
2	Atomistic Models	9
2.1	Friction Models	9
2.2	Physical Essence of Mechanical Adiabaticity in Friction	11
3	Atomistic Locking and Friction	15
3.1	Theoretical Preliminaries	15
3.1.1	Model	15
3.1.2	Expression for Adiabatic Potential	17
3.2	Topological Description of Friction	19
3.2.1	Adiabatic Potential	19
3.2.2	Atomic Configurations of Surfaces	19
3.2.2.1	Variant $\bar{P}_\gamma(\rho)$ Case	21
3.2.2.2	Invariant $\bar{P}_\gamma(\rho)$ Case	22
3.2.2.3	Restricted Invariant $\bar{P}_\gamma(\rho)$ Case	22
3.3	A More Realistic Case: A Relaxed Upper Body	22
3.4	Quasi-static Friction of α -Iron	24
3.4.1	Case (a)	24
3.4.2	Case (b)	25
4	Atomistic Origin of Friction	29
4.1	Friction Model	29
4.2	Static Friction	31
4.3	Energy Dissipation in Dynamic Friction	32
4.4	Criterion for Friction Transition	35

5	Superlubricity	43
5.1	A State of Vanishing Friction	43
5.2	How Does Friction Become Zero?	44
5.3	Nonadiabatic Motion of Atoms	45
5.4	Importance of High Dimensionality	46
6	Atomistic Simulation of Friction	49
6.1	Computer Simulation	49
6.2	Atomic Structure and Electronic States	51
6.2.1	Properties of Atoms	51
6.2.2	Electronic States	53
6.3	Cohesion of Solids	55
6.3.1	Cohesive Forces Between Molecules	55
6.3.2	Cohesive Forces in Solids	58
6.4	Crystal Binding	58
6.4.1	Ionic Crystals	59
6.4.2	Covalent Crystals	60
6.4.3	Metallic Crystals	61
6.4.4	Molecular Crystals	62
6.4.5	Hydrogen-Bonded Crystals	64
6.5	Interatomic Force and Interatomic Potential	66
6.6	Molecular Dynamics Method	68
6.6.1	Equations of Motion of Atoms	68
6.6.2	Numerical Integral	68
6.7	Simple Atomistic Model	69
6.7.1	Friction Model	69
6.7.2	Equation of Motion in Dimensionless Form	70
6.7.3	Friction Diagram	72
6.8	Energy Recurrence in Superlubricity	75
6.8.1	Energy Dissipation	75
6.8.2	Two-Dimensional Model Simulation	76
6.9	Realistic Systems	79
6.9.1	Friction Transition	79
6.9.2	Many-Body Interatomic Potentials	80
6.9.3	Stability of Superlubricity	82
7	Experimental Approach for Atomic Level Friction	85
7.1	Atomic Force Microscopy Techniques	85
7.2	Verification of Atomistic Theory	87
7.2.1	Static Friction Forces	87
7.2.2	Commensurability in Sliding Surfaces	88
8	Summary	99
8.1	Origin of Friction	99
8.2	Controlling Friction	100

A	Physical Preliminaries	103
A.1	Analytical Mechanics	103
A.1.1	Coordinates and Transformation of a Coordinate System	103
A.1.1.1	Cartesian Coordinate System	104
A.1.1.2	Expression of Velocity and Acceleration in Polar Coordinates	104
A.1.1.3	Three-Dimensional Polar Coordinate System	108
A.1.1.4	Cartesian Curvilinear Coordinates	111
A.1.1.5	Generalized Coordinates	113
A.1.1.6	Generalized Momentum and Canonical Conjugate Variable	116
A.1.1.7	Generalized Force	116
A.1.2	Lagrange Equation of Motion and Variational Principle	118
A.1.2.1	Lagrange Equation of Motion	118
A.1.2.2	Application of Lagrange's Equation of Motion	120
A.1.2.3	Variational Principle and Euler–Lagrange Equation	123
A.1.2.4	Principle of Virtual Work	126
A.1.3	Hamilton's Canonical Equation	129
A.1.3.1	Hamiltonian	129
A.1.3.2	Hamilton's Canonical Equation	132
A.1.3.3	Phase Space and Trajectory of Motion	132
A.2	Fundamentals of Statistical Mechanics	134
A.2.1	Kinetic Theory of Gases	134
A.2.2	Principle of Equal <i>a priori</i> Probability and Ergodic Hypothesis	138
A.2.3	Microscopic State	139
A.2.4	Number of States and Density of States	142
A.2.5	Entropy	144
A.2.6	Thermal Equilibrium of a Coupled System	145
A.2.7	Constant Temperature System: Canonical Ensemble	148
A.2.8	Classical System at a Given Temperature	152
A.3	Classical Mechanics with Vector Analysis	154
A.3.1	Law of Motion	154
A.3.2	Motion of Mass Point Expressed with a Vector	155
A.3.3	Moment of Force Acting on Mass Point	157
A.3.4	Angular Velocity Vector	157
A.3.5	Outer Product and Rotation	158
A.4	Vibration and Wave	159
A.4.1	What is a Wave?	159
A.4.2	Fundamental Relation	161
A.4.3	Harmonic Oscillation	162
A.4.4	Wave Function	164
A.4.5	Wave Equation	167
A.4.6	Traveling Wave	169
A.4.7	Phase Velocity and Dispersion	170
A.4.8	Group Velocity	172
A.4.9	Three-Dimensional Wave: Plane Wave	175
A.5	Lattice Vibration	179

A.5.1	Lattice Vibration and Thermal Properties of Crystals	179
A.5.2	Lattice Vibration of a One-Dimensional Crystal	184
A.5.2.1	Model of a One-Dimensional Crystal	184
A.5.2.2	Continuum Approximation	185
A.5.2.3	Natural Vibration and Natural Frequency	187
A.5.2.4	Dispersion Relation	189
A.5.2.5	First Brillouin Zone	189
A.5.3	Acoustical Mode and Optical Mode	191
A.5.4	Lattice Vibration in a Three-Dimensional Crystal	196
A.5.5	Phonon	197

B Mathematical Supplement 199

B.1	Trigonometry	199
B.1.1	Definition	199
B.1.2	Addition Formula	200
B.1.3	Basic Properties	202
B.2	Taylor Expansion	204
B.3	Complex Exponential Function	206
B.4	Vectors and Geometry	208
B.4.1	Equations of Line and Plane	208
B.4.1.1	Equations of Line	208
B.4.1.2	Equation of a Plane	209
B.4.1.3	Equation of a Sphere and a Spherical Tangent Plane	214
B.4.1.4	Application to Geometry	215
B.5	Linear Algebra	216
B.5.1	Determinant and Inverse Matrix	216
B.5.1.1	Permutation	216
B.5.1.2	Definition of a Determinant	217
B.5.1.3	Characteristics of a Determinant	217
B.5.1.4	Inverse Matrix	218
B.5.1.5	Application of a Determinant	219
B.5.2	Linear Equations: Cramer's Formula	219
B.5.3	Eigenvalue and Eigenvector	221
B.5.3.1	Eigenvalue and Eigenvector of a Square Matrix	221
B.5.3.2	Diagonalization of a Matrix	223
B.5.3.3	Normal Form of a Quadratic Form Polynomial	225

C Data Analysis 227

C.1	Fundamentals of Description of Physical Data	227
C.1.1	Classification of Deterministic Data	228
C.1.1.1	Sinusoidal Periodic Data	228
C.1.1.2	Compound Periodic Data	229
C.1.1.3	Almost Periodic Data	232
C.1.2	Classification of Random Data	233
C.1.2.1	Stationary Irregular Process	233
C.1.2.2	Ergodic Irregular Process	234

C.1.3	Fundamental Properties of Random Data	235
C.1.3.1	Squared Average: Average and Variance	235
C.1.3.2	Probability Density Function	235
C.1.3.3	Autocorrelation Function	237
C.1.3.4	Power Spectral Density Function	237
C.2	Signal Processing	239
C.2.1	Analog Signal and Digital Signal	239
C.2.2	Fourier Analysis	240
C.2.2.1	Fourier Series	240
C.2.2.2	Fourier Transform	242
C.2.2.3	Discrete Fourier Transform	243
C.2.3	Applications of Fourier Transform	246
C.2.3.1	Impulse Response	246
C.2.3.2	Analysis of a Linear System	250
C.2.3.3	Equation of Motion	252
D	Crystal Structure	255
D.1	Periodicity of Crystals	255
D.2	Crystal Structure	256
D.2.1	Simple Cubic Structure	256
D.2.2	Body-Centered Cubic Structure	256
D.2.3	Face-Centered Cubic Structure	257
D.2.4	Hexagonal Closed-Packed Structure	258
D.2.5	Sodium Chloride Structure and Cesium Chloride Structure	259
D.2.6	Diamond Structure	260
D.3	X-ray Diffraction	261
D.3.1	Diffraction Condition	261
D.3.2	Reciprocal Vector	263
D.3.3	Bragg's Condition	264
D.4	Various Crystal Data	264
E	The SI (mks) Unit System	267
E.1	Three Basic Units	267
E.1.1	Unit of Length: Meter	267
E.1.2	Unit of Time: Second	268
E.1.3	Unit of Mass: Kilogram	268
E.1.3.1	Atomic Mass Unit	268
E.2	The SI (mks) Unit System	269
E.3	The cgs System	273
F	Practice for Verlet Algorithm	275
G	Program Example of Molecular Dynamics for Atomistic Model	279
G.1	Annealing Program	279
G.2	Sliding Program	281

H **Table of Values** 285

I **Table of Relative Atomic Weights** 287

References 289

Afterword 295

About the Author 297

Index 299