

CONTENTS

Preface	v
1 Background and Some Concepts	1
1.1. Elastic and Plastic Regimes	1
1.1.1. Elastic Deformation	1
1.1.2. Atomic Forces and Elastic Properties	2
1.1.3. Plastic Deformation	3
1.2. Griffith Criterion: Role of Surfaces	4
1.3. Peierls Stress and Barrier	6
1.4. Dislocation Core and Atomic Force	8
1.5. Stacking Faults	8
1.6. Glissile and Sessile Dislocations	9
1.7. Concept of Fractals	9
1.8. 'Glue' and Related Models of Interatomic Force Fields	10
1.9. Pair Potentials	11
1.10. Grain and Twin Boundaries	11
1.11. Alloy Formation: Rules and Models	12
1.11.1. Solid Solubility: Hume-Rothery Factors	12
1.12. Friction Mechanisms	16
2 Phenomenology and Experiments	19
2.1. Plastic Deformation of bcc Metals	20
2.1.1. Deviation from the Schmid Law	20
2.1.2. Temperature Dependence of Critical Resolved Shear Stress of bcc Metals	21
2.2. Phonons, Electrons and Plasticity	25
2.2.1. Phonon Drag of Dislocations in Metals	26
2.2.2. Electron Drag of Dislocations in Metals	26
2.2.3. Superconductivity and Plasticity	27
2.2.4. The Electroplastic Effects in Metals	30
2.3. High Temperature Strength of Alloys	31
2.3.1. Diffusion Creep	31
2.3.2. Effect of Solute Atoms	33

2.4.	The Crack and Fracture	34
2.4.1.	Cleavage Cracks	34
2.4.2.	Emitting Cracks	34
2.4.3.	Plastically Blunted Cracks	34
2.4.4.	The Condition for Intrinsic Brittleness	35
2.4.5.	Dislocation Shielding, Antishielding and Annihilation at the Crack Tip	36
2.4.6.	Dislocation Dynamics and Fracture	37
2.5.	Power Law Relation between the Plastic Strain and the Number of Cycles to Fatigue Failure	38
2.6.	Statistical Behaviour for the Fracture of Disordered Media	38
2.6.1.	Statistical Fluctuations in the Rupture Stress of Materials	39
2.6.2.	The Dependence of the Mean Fracture Stress on the Sample Size	39
2.6.3.	Local Damage Zones	39
2.7.	The Roughness of the Crack Surface	41
2.8.	Dynamic Instabilities of Fracture	41
3	Introduction to Extended Defects and Mechanical Strength	43
3.1.	Some Basic Theory of Crystal Dislocations	43
3.1.1.	Dislocations and Slip	43
3.1.2.	Burgers Vector	45
3.1.3.	Glide and Climb	46
3.1.4.	Jogs	47
3.1.5.	Forces on Dislocations	48
3.2.	Elastic Field of Straight Dislocation	48
3.2.1.	Summary of Isotropic Elasticity Theory	49
3.2.2.	Elastic Field of An Edge Dislocation	51
3.2.3.	Elastic Field of Screw Dislocation	53
3.2.4.	Uniform Dissociation Model of Dislocation Core	54
3.2.5.	Mixed Dislocations	57
3.2.6.	Dislocations in Anisotropic Media	57
3.3.	Interactions of Dislocation with Other Defects	57
3.3.1.	Interactions with Point Defects	57
3.3.2.	Interactions with Planar Free Surface	59
3.4.	Crystal Lattice Effects	60
3.4.1.	Stacking Order in Closed-Packed Structures	60
3.4.2.	Partial and Extended Dislocations in fcc Crystals	61
3.4.3.	Stacking Faults and Extended Dislocations in Plastic Deformation	61
3.5.	Dislocation Motion over Peierls Barrier	62
3.5.1.	Peierls Model	63
3.5.2.	Frenkel-Kontorova Model	63

3.5.3. Phase Transition: Analytical Mechanism Motion of Dislocations	64
3.5.4. Dislocation Velocity	66
3.5.5. Quantum Motion of Dislocations	67
3.5.6. Flow Limit	67
3.6. Dislocations and Cracks	69
3.6.1. Fundamental Properties of Dislocation Arrays	70
3.6.2. Solution of Integral Equation with Chebyshev Polynomials	72
3.6.3. Elastic Energy Momentum Tensor in Defect Problem	73
3.6.4. Gauge Field Theory of Defects	78
3.6.5. Interactions of Dislocations with Crack	82
3.6.6. Dislocation Distribution Function in Plastic Zone at Crack Tip	86
3.6.7. Dislocation Emission from Cracks	91
3.6.8. Dislocation Pair Creation and Separation from the Crack Tip	94
3.6.9. Dislocation Free Zone at Crack Tip	96
3.7. Geometrical Aspects of Grain Boundaries	102
3.7.1. $\Sigma = 3$ Tilt Boundary with a $\langle 112 \rangle$ Rotation Axis in Cu	103
3.7.2. Grain Boundary Phases in Copper-Bismuth Alloys	104
3.7.3. Grain Boundary in NiAl with N-body Empirical Potentials	106
3.7.4. Example (Schematic) of Low-Energy Grain-Boundary Structure as Determined by Atomistic Simulation	107
3.8. Creep: Example of Single Crystal of Lead	108
3.9. Superplastic Materials	110
3.10. Mechanical Properties of Fatigued fcc Crystals and their Dislocation Arrangements	110
4 Some Characteristic Features of Fractals	113
4.1. Self-Similarity and Fractals	113
4.2. Self-Similarity and Dimension	116
4.3. Hausdorff-Besicovitch Dimension	117
4.4. The Koch Curves	120
4.5. The Cantor Set	122
4.6. The Residual Set and "Fat Fractals"	125
4.7. Statistical Self-Similarity	126
4.8. Brownian Motion and Time Series	127
4.9. Self-Similarity and Self-Affinity	129
4.10. The Relation of D to H	130
4.11. Multifractal Measures	133
4.12. Percolation Models of Breakdown	136
4.13. Fractal Description of Fractures	137
4.13.1. Slit-island Method (SIM) and Difficulties	140
4.13.2. The Roughness Exponent	145

4.14.	Multirange Fractals in Materials	149
4.15.	Time Evolution of Multirange Fractals	158
4.16.	Fragmentation	160
	4.16.1. Equal-Ratio-Edged Orthorhombic Fragments Model (ERE)	162
	4.16.2. Volume-scaling Fragmentation (VSF)	165
4.17.	Phenomenological Relation Between Fractal Dimension of Fractured Surfaces and Fracture Toughness of Materials	168
	4.17.1. Universality and Specificity of Fractures	168
	4.17.2. Linear Elastic Fracture	169
	4.17.3. Quasi-brittle Fracture	174
4.18.	Physical Sources of Fractal Surfaces	181
	4.18.1. Intergranular Fracture Model	181
	4.18.2. Transgranular Fracture Model	185
	4.18.3. Changes in Fracture Mechanism	185
	4.18.4. Fractal Crack Growth	186
	4.18.5. Dynamic Instability	188
	4.18.6. Evolution Induced Catastrophic Model	189
	4.18.7. Oscillatory Propagation of a Slant Crack	189
5	Elastic Moduli and More General Phonon Properties	193
5.1.	Outline	193
5.2.	Force between Half-Planes of a Metal	193
	5.2.1. Relation of Cleavage Force to Surface Energy of Metal	194
	5.2.2. Kohn-Yaniv Interpolation Formula for Cleavage Force	195
	5.2.3. Universal Model for Cleavage Force	196
	5.2.4. Emission of Phonons by Moving Dislocations	197
	5.2.5. Effect of Stress and Temperature on Velocity of Dislocations in Fe Single Crystals	198
	5.2.6. Pair Potential: Uses and Limitations	198
	5.2.7. Some Useful Combinations of Elastic Constants for Hexagonal Close Packed Metals	199
5.3.	Empirical Relations between Elastic Moduli, Vacancy Formation Energy and Melting Temperature	200
6	Elements of Electronic Structure Theory	203
6.1.	Free Electron Theory	203
	6.1.1. Bulk Moduli of Metals Compared with Free Electron Model	204
6.2.	Exchange and Correlation Interactions	205
	6.2.1. Exchange Hole	205
6.3.	Bulk Modulus Including Exchange and Correlation	207
6.4.	Structural Stability of Non-Transition Metals	208
	6.4.1. Trends Along Columns in Periodic Table	211

6.5. Elastic Constants of Hexagonal Transition Metals from Electronic Structure Calculations	213
6.5.1. Cauchy Relations for Central Forces	213
6.5.2. Results for an Isotropic Medium	215
6.5.3. Changes in Electronic Density of States for Various Strains	215
6.6. Energy of Simple Metals as Volume Term Plus Pair Potential Contribution	215
6.7. Pair Potentials	216
6.8. Structural Stability of Transition Metals	217
6.9. Electron Density in Interstitial Region in Metals	220
6.10. Trends in Vacancy Formation Energy with d-Shell Filling in Transition Metals	221
6.11. Bloch's Theorem and Energy Bands	222
6.12. Pseudopotentials	224
6.13. Coordination Dependent and Chemical Models	226
6.13.1. Metal Clusters	226
6.13.2. Binary Metallic Alloys	227
6.13.3. Structure and Bonding of Fe ₃ Al and FeAl	227
7 Theory of Pair Potentials in Simple s-p Metals	231
7.1. Thomas-Fermi Theory of Interaction Between Test Charges in Initially Uniform Electron Gas	231
7.1.1. Test Charge Interaction Energy: Basis of Electrostatic Model	232
7.1.2. Wave Theory of Interaction Between Test Charges	232
7.2. Density Functional Theory of Pair Potentials	238
7.2.1. Density Functional Theory of Pair Potential	240
7.2.2. Solution of One-Centre Problem for Na Atom Embedded in a Cavity in Jellium	241
7.2.3. Pair Interaction Between Ions	242
7.2.4. Inversion of Measured Liquid Structure Factor $S(k)$ for Na Near Melting to Extract a 'Diffraction' Pair Potential	245
7.2.5. Approximate Analytic Structural Theories	246
7.2.6. Pair Potentials for Iridium and Rhodium	247
7.2.7. Structure and Properties of Dislocations	250
8 Transcending Pair Potentials: Glue Models of Interatomic Forces	251
8.1. Introduction	251
8.2. Embedded Atom and Related Approaches	251
8.2.1. First-Principles Energy Calculations for Al Structures	252
8.2.2. Coordination Number Dependence of Energy/Atom for Al Structures	252

8.2.3. Methodology	253
8.3. Embedded Atom Method: Analytic Model for fcc Metals	254
8.3.1. Average Shear Constant	255
8.3.2. Analytic Results for Vacancy and Divacancy Energetics	255
8.3.3. Hexagonal-Close-Packed Metals	256
8.4. Inequality Relating Vacancy Formation Energy in a Hot Crystal (Near Melting to Rigidity)	257
8.5. Screw Dislocation Core Structures for Niobium and Molybdenum	259
8.6. Quantum-Chemical Model of Cold Metallic Lattice Energies as Function of Coordination Number c	261
8.7. Further Work on Dislocations and Grain Boundaries	262
8.7.1. Body-Centred Cubic Metals	262
8.7.2. Grain Boundaries in Metals and Alloys	263
8.8. Friction, Mechanical Properties and Interatomic Interactions	266
8.9. Empirical Potentials vs Density Functional Calculations for Mechanical Properties	267
9 Positron Annihilation: Experiment and Theory	269
9.1. Background	269
9.2. Interaction of Positrons with Vacancies in Metals	270
9.3. Trapping Model	273
9.3.1. Positron-Diffusion Mechanism and Enthalpy of Formation of Monovacancies	275
9.3.2. Trapping Rate	278
9.4. Positron-Annihilation Characteristics	279
9.4.1. Vacancies and Vacancy Clusters	281
9.4.2. Dislocations	287
9.4.3. Grain Boundaries and Interfaces	292
9.4.4. Voids and Cracks	298
9.5. Electron and Positron Momentum Distributions in Solids	300
9.5.1. Introduction	300
9.5.2. Positron Implantation and Thermalization	301
9.5.3. Positron Diffusion	303
9.5.4. Positron Distribution in Solids	304
9.5.5. Electron-Positron Correlation in Pure Metals and the Core Effects	306
9.5.6. Momentum Density in Crystalline Solids	308
9.5.7. 1D and 2D ACAR Measurements	309
9.5.8. Examples of Momentum Density Calculations and Experiments	311
9.6. Experimentation with Low-Energy Positron Beams	314
9.6.1. Positron Diffusing Back to Metal Surface	315
9.6.2. Positron Trapping at Monovacancies Near a Surface	315

9.6.3. Defect Profiling with Positron-Beams	316
9.7. Summary	317
10 Stretched Chemical Bonds, Electron Correlation and Extended Defect Propagation	319
10.1. Roughness and Toughness of Metals and Metallic Alloys	319
10.2. Perfect Crystal Properties: Elastic Constants and Melting Points	323
10.2.1. Bonding Energies of Metals	232
10.2.2. Melting Energies	323
10.2.3. Interatomic Forces in Solid Solution of Transition Metal Alloys	328
10.2.4. Bonding Characteristic of Ni ₃ Al	330
10.2.5. The Empirical Electron Theory of Solids (EET) and The Brittleness of σ -Phase in Fe-Cr Alloys	331
10.3. Morse Potentials and crss of Iron Single Crystals	332
10.4. Plastic Deformation of L1 ₂ Ordered Alloys	341
10.5. Breaking-Bond Models of Propagation of Extended Defects	342
10.5.1. Stretched Chemical Bond in H ₂ and Electron Correlation	343
10.5.2. Cleavage Force in Directionally Bonded Solids	344
10.5.3. Steady-State Propagation of Screw Dislocation in a Bond-Breaking Model	344
10.5.4. Unified Treatment of Lattice Dynamical Models of a Crack and of a Screw Dislocation	347
10.6. Grain Boundaries (GB), Plastic Behaviour and Fracture	349