THE PHYSICS AND CHEMISTRY OF MATERIALS
For Harriet and Françoise
CONTENTS

PREFACE xxi

LIST OF TABLES xxvii

Introduction 1

SECTION I STRUCTURE OF MATERIALS

1 Structure of Crystals 5
   1.1 Introduction 5
   Introduction to Lattices 6
   1.2 Translation Vectors 6
   1.3 Unit Cells 8
   1.4 Bravais Lattices 8
   1.5 Lattice Axes, Planes, and Directions 11
   Local Atomic Bonding Units and Crystal Structures 14
   1.6 Local Atomic Bonding Units 15
   1.7 Crystal Structures 20
   1.8 Packing Fractions and Densities 32
   References 34
   Problems 35

W1.1 Crystal Structures Based on Icosahedral Bonding Units
W1.2 Packing Fractions of BCC and CsCl Crystal Structures
W1.3 Density of CsCl
Problem

2 Bonding in Solids 37
   2.1 Introduction 37
   Bonding in Elemental Solids 39
   2.2 Covalent Bonding 40
   2.3 Metallic Bonding 44
   2.4 van der Waals Bonding 45
   Bonding in Multielement Crystals 47
   2.5 Ionic Bonding 48
   2.6 Mixed Ionic–Covalent Bonding and Ionicity 53
   2.7 Hydrogen Bonding 53

vii
<table>
<thead>
<tr>
<th>CONTENTS</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Cohesive Energies</td>
<td>54</td>
</tr>
<tr>
<td>Summary of Some Atomic Properties and Parameters</td>
<td>57</td>
</tr>
<tr>
<td>2.8 Ionization Energy and Electron Affinity</td>
<td>58</td>
</tr>
<tr>
<td>2.9 Electronegativity</td>
<td>58</td>
</tr>
<tr>
<td>2.10 Atomic Radii: Ionic, Covalent, Metallic, and van der Waals</td>
<td>60</td>
</tr>
<tr>
<td>References</td>
<td>65</td>
</tr>
<tr>
<td>Problems</td>
<td>65</td>
</tr>
<tr>
<td>W2.1 Atomic, Hybrid, and Molecular Orbitals Involved in Bonding in Solid-State Materials</td>
<td></td>
</tr>
<tr>
<td>W2.2 Absence of Covalent Bonding in White Sn (β-Sn) and Pb</td>
<td></td>
</tr>
<tr>
<td>W2.3 Madelung Energy of Ionic Crystals</td>
<td></td>
</tr>
<tr>
<td>W2.4 Hydrogen Bonding in Ice (Solid H₂O)</td>
<td></td>
</tr>
<tr>
<td>W2.5 Standard Enthalpies of Formation</td>
<td></td>
</tr>
<tr>
<td>W2.6 Bond Energies</td>
<td></td>
</tr>
<tr>
<td>W2.7 Ionization Energies and Electron Affinities</td>
<td></td>
</tr>
<tr>
<td>W2.8 Valence</td>
<td></td>
</tr>
<tr>
<td>W2.9 Electronegativity</td>
<td></td>
</tr>
<tr>
<td>W2.10 Atomic Radii</td>
<td></td>
</tr>
<tr>
<td>References</td>
<td></td>
</tr>
<tr>
<td>Problems</td>
<td></td>
</tr>
<tr>
<td>3 Diffraction and the Reciprocal Lattice</td>
<td>67</td>
</tr>
<tr>
<td>Diffraction</td>
<td></td>
</tr>
<tr>
<td>3.1 Fourier Analysis in One and Three Dimensions</td>
<td>68</td>
</tr>
<tr>
<td>3.2 Examples of Reciprocal Lattices</td>
<td>71</td>
</tr>
<tr>
<td>Elastic Scattering from Ordered and Disordered Materials</td>
<td>73</td>
</tr>
<tr>
<td>3.3 Crystalline Solids</td>
<td>75</td>
</tr>
<tr>
<td>3.4 Bragg and von Laue Descriptions of Diffraction</td>
<td>77</td>
</tr>
<tr>
<td>3.5 Polycrystalline Solids or Powders</td>
<td>78</td>
</tr>
<tr>
<td>3.6 Elastic Scattering from an Amorphous Solid</td>
<td>81</td>
</tr>
<tr>
<td>References</td>
<td>82</td>
</tr>
<tr>
<td>Problems</td>
<td>83</td>
</tr>
<tr>
<td>W3.1 Voronoi Polyhedra</td>
<td></td>
</tr>
<tr>
<td>W3.2 Molecular Geometry and Basis Structure from Diffraction Data</td>
<td></td>
</tr>
<tr>
<td>Reference</td>
<td></td>
</tr>
<tr>
<td>Problem</td>
<td></td>
</tr>
<tr>
<td>4 Order and Disorder in Solids</td>
<td>85</td>
</tr>
<tr>
<td>4.1 Introduction</td>
<td>85</td>
</tr>
<tr>
<td>Order and Disorder</td>
<td>86</td>
</tr>
<tr>
<td>4.2 Examples of Ordered and Disordered Solids</td>
<td>91</td>
</tr>
<tr>
<td>4.3 Amorphous Solids</td>
<td>96</td>
</tr>
</tbody>
</table>
Defects in Solids
4.4 Localized Defects 103
4.5 Extended Defects 106
4.6 Thermodynamics of Defect Formation: Entropy 111
4.7 Examples of Defect Studies 115
References 117
Problems 117

W4.1 Further Discussion of the Random Close-Packing Model
W4.2 Further Discussion of the Continuous Random Network Model
W4.3 Illustrations of the Law of Mass Action
W4.4 Nonstoichiometry
Reference

SECTION II PHYSICAL PROPERTIES OF MATERIALS

5 Phonons 121
Excitations of the Lattice: Phonons 121
5.1 One-Dimensional Monatomic Lattice 122
5.2 One-Dimensional Diatomic Lattice 126
5.3 Phonons: General Case 128
5.4 Phonon Density of States 130
Lattice Specific Heat of Solids 133
5.5 Specific Heat of Solids 134
5.6 Debye Theory of Specific Heat 135
5.7 Einstein Theory of Specific Heat 138
5.8 Debye–Waller Factor 139
Anharmonic Effects 139
5.9 Thermal Expansion 140
5.10 Thermal Conductivity 144
References 150
Problems 151

W5.1 Monatomic Lattice with Random Interactions
W5.2 Debye–Waller Factor
Appendix W5A: Quantization of Elastic Waves
Appendix W5B: Dispersion Relations in the General Case
Appendix W5C: Van Hove Singularities

6 Thermally Activated Processes, Phase Diagrams, and Phase Transitions 153
6.1 Introduction 153
Thermally Activated Processes 153
CONTENTS

7.19 Landauer Theory of Conduction 228

References 229

Problems 229


W7.1 Boltzmann Equation
W7.2 Random Tight-Binding Approximation
W7.3 Kronig–Penney Model
W7.4 Hall Effect in Band Theory
W7.5 Localization
W7.6 Properties of Carbon Nanotubes

Appendix W7A: Evaluation of Fermi Integrals

8 Optical Properties of Materials 231

8.1 Introduction 231
8.2 The Electromagnetic Spectrum 232
8.3 AC Conductivity of Metals 233
8.4 Reflectivity 234
8.5 Optical Properties of Semiconductors 241
8.6 Optical Dielectric Function 243
8.7 Kramers–Kronig Relations 245
8.8 Optical Properties of Composite Media 246
8.9 Nonlinear Polarization 247
8.10 Excitons 250
8.11 Color Centers 253
8.12 Polaritons 254
8.13 Emissivity 254

References 258

Problems 258


W8.1 Index Ellipsoid and Phase Matching
W8.2 Polaritons

Appendix W8A: Maxwell’s Equations
Appendix W8B: Nonlocal Dielectric Function
Appendix W8C: Quantum-Mechanical Derivation of the Dielectric Function

9 Magnetic Properties of Materials 261

9.1 Introduction 261

Origins of Magnetism in Solids 261
9.2 Free Atoms and Ions 261
9.3 Atoms and Ions in Solids 266

Types of Magnetism and Magnetic Behavior in Materials 276
9.4 Paramagnetism 278
9.5 Interactions Between Magnetic Moments 283
9.6 Ferromagnetism 287
CONTENTS

9.7 Antiferromagnetism 297
9.8 Ferrimagnetism 301
9.9 Magnetic Behavior of Electrons in Closed Shells and of Conduction Electrons 304

References 309
Problems 309

W9.1 Jahn–Teller Effect
W9.2 Examples of Weak and Strong Crystal Field Effects
W9.3 Crystal Fields and Cr^{3+} in Al_{2}O_{3}
W9.4 Experimental Results for \chi in the Free-Spin Limit
W9.5 Spin Glasses and the RKKY Interaction
W9.6 Kondo Effect and s–d Interaction
W9.7 \chi(T) for Ni
W9.8 Hubbard Model
W9.9 Microscopic Origins of Magnetocrystalline Anisotropy
W9.10 \chi|| and \chi\perp for Antiferromagnetic Materials
W9.11 Magnetism in Disordered Materials

References
Problems

10 Mechanical Properties of Materials 311

10.1 Introduction 311

Stress, Strain, and Elastic Constants 311

10.2 Stress 312
10.3 Strain 314
10.4 Relationships Between Stress and Strain: Elastic Constants 317

Elastic Properties of Materials 320

10.5 Hooke’s Law, Young’s Modulus, and Shear Modulus 320
10.6 Compressibility and Bulk Modulus 323
10.7 Poisson’s Ratio 324
10.8 Isotropic Solids: Relationships Between the Elastic Moduli 325
10.9 Elastic Potential Energy 326
10.10 Elastic Waves 327

Anelastic Properties of Materials 330

10.11 Macroscopic Aspects of Anelasticity 330
10.12 Microscopic Aspects of Anelasticity 332

Inelastic Properties of Materials 334

10.13 Macroscopic Aspects of Plasticity and Fracture 335
10.14 Microscopic Aspects of Plasticity and Fracture 341

References 351
Problems 351

W10.1 Relationship of Hooke’s Law to the Interatomic \Upsilon(r)
W10.2 Zener Model for Anelasticity
CONTENTS

W10.3 Typical Relaxation Times for Microscopic Processes
W10.4 Further Discussion of Work Hardening
W10.5 Strengthening Mechanisms
W10.6 Creep Testing
W10.7 Further Discussion of Fatigue
W10.8 Hardness Testing
W10.9 Further Discussion of Hall–Petch Relation
W10.10 Analysis of Crack Propagation

Reference
Problems

SECTION III CLASSES OF MATERIALS

11 Semiconductors 357

11.1 Introduction 357
Characteristic Properties of Semiconductors 357
Microscopic Properties 359
11.2 Energy-Band Structure and Energy Gaps 359
11.3 Dynamics of Electron Motion 366
11.4 Excited States of Electrons 367
11.5 Doping and Defects 374
11.6 Dimensionality and Quantum Confinement 382
Macroscopic Properties 387
11.7 Electrical Conductivity and Mobility 388
11.8 Effects of Magnetic Fields 394
11.9 Optical Properties 396
Examples of Semiconductors 404
11.10 Elemental Semiconductors and Their Compounds and Alloys 405
11.11 Compound Semiconductors and Their Alloys 409
Applications of Semiconductors 419
11.12 Critical Issues 419
11.13 Specific Applications 434
References 439
Problems 440

W11.1 Details of the Calculation of $n(T)$ for an n-Type Semiconductor
W11.2 Effects of Doping on Resistivity of Silicon
W11.3 Optical Absorption Edge of Silicon
W11.4 Thermoelectric Effects
W11.5 Dielectric Model for Bonding
W11.6 Nonstandard Semiconductors
W11.7 Further Discussion of Nonequilibrium Effects and Recombination
W11.8 Transistors
W11.9 Quantum Hall Effect
W11.10 Photovoltaic Solar Cells
W11.11 Thermoelectric Devices
Appendix W11A: Landau Levels
References
Problems

12 Metals and Alloys

12.1 Introduction 443
Three Classes of Metals 444
12.2 $sp$-Bonded Metals 444
12.3 Transition Metals 449
12.4 Rare Earth Metals 451
Alloys 452
12.5 Hume–Rothery Rules 453
12.6 Electrical Resistance of Metallic Alloys 455
Examples and Applications of Metallic Alloys 457
12.7 Steel 457
12.8 Intermetallic Compounds and Superalloys 458
12.9 Electromigration 462
References 463
Problems 464

W12.1 Density-Functional Theory
W12.2 Embedded-Atom Method
W12.3 Peierls Instability
W12.4 Corrosion and Oxidation
W12.5 Coatings
W12.6 Shape-Memory Alloys
W12.7 Metallic Glasses
W12.8 Metal Hydrides
W12.9 Solder Joints and Their Failure
W12.10 Porous Metals
References

13 Ceramics

13.1 Introduction 465
13.2 Pauling Bonding Rules 467
13.3 Ionic Interactions 469
Applications 471
13.4 Refractories 471
13.5 Silicon Nitride 475
13.6 Zeolites 477
13.7 Glasses 481
References 488
14 Polymers 491

14.1 Introduction 491
Structure of Polymers 492

14.2 Geometry of Polymers 495
14.3 Polymer Crystals 497
14.4 Defects in Polymers 498

Mechanical Properties 501

14.5 Polymers Under Tension 502
14.6 Viscoelasticity 506

Thermal Properties 510

14.7 Thermal Properties of Polymers 510
Applications 514

14.8 Structural Plastics 514
14.9 Polymeric Ionic Conductors 515
14.10 Photoresists 516
14.11 Piezoelectric Polymers 517
14.12 Liquid Crystals 519

References 522
Problems 523


W14.1 Structure of Ideal Linear Polymers
W14.2 Self-Avoiding Walks
W14.3 Persistence Length
W14.4 Free-Volume Theory
W14.5 Polymeric Foams
W14.6 Porous Films
W14.7 Electrical Conductivity of Polymers
W14.8 Polymers as Nonlinear Optical Materials

Problems

15 Dielectric and Ferroelectric Materials 525

15.1 Introduction 525
15.2 Lorentz Oscillator Model for the Dielectric Function 525
15.3 Dielectric Properties of Ionic Crystals 529
15.4 Dielectric Breakdown 530
Applications 533
15.5 Ferroelectric Phase Transitions 533
15.6 Ferroelectricity and Piezoelectricity 536
15.7 Thermistors 541
15.8 Varistors 543
15.9 $\beta$-Aluminas and Ionic Transport in Solids 545
References 547
Problems 547

Topics at the Web Site (ftp://ftp.wiley.com/public/sci...med/materials)
W15.1 Capacitors
W15.2 Substrates
W15.3 First-Order Ferroelectric Phase Transitions
W15.4 Nonvolatile Ferroelectric Random-Access Memory
W15.5 Quartz Crystal Oscillator
W15.6 Lithium-Ion Battery
W15.7 Fuel Cells
References
Problem

16 Superconductors 549

16.1 Introduction 549
Characteristic Properties of Superconductors 550
16.2 Macroscopic Properties and Models 551
16.3 Microscopic Properties and Models 571
Examples of Superconductors 581
16.4 Metallic Elements 581
16.5 Oxide-Based Ceramics 582
Applications of Superconductors 589
16.6 Critical Issues 589
16.7 Specific Applications 595
References 599
Problems 599

Topics at the Web Site (ftp://ftp.wiley.com/public/sci...med/materials)
W16.1 Further Discussion of Thermal Conductivity in Superconductors
W16.2 Two-Fluid Model
W16.3 Superconducting Alloys of Metallic Elements
W16.4 Superconducting Intermetallic Compounds
W16.5 Further Discussion of Structure, Bonding, Composition, and Normal-State Properties of the Oxide-Based Ceramic Superconductors
W16.6 Further Discussion of Superconducting-State Properties of the Oxide-Based Ceramic Superconductors
W16.7 Unusual Superconductors
W16.8 Further Discussion of Critical Currents
17 Magnetic Materials 603

17.1 Introduction 603
Characteristic Properties of Magnetic Materials 603

17.2 Magnetic Microstructure and Domains 604
17.3 Magnetization Processes and Magnetization Curves 611
17.4 Magnetically Hard and Soft Materials 616
17.5 Effects of Magnetic Anisotropy 617
17.6 Effects of Shape and Size 620

Important Effects in Magnetic Materials 622

17.7 Magnetostriction 623
17.8 Magnetoresistance 626
17.9 Magneto-Optical Effects 627
17.10 Dynamic Magnetic Effects 628

Examples and Applications of Magnetic Materials 629

17.11 Hard Magnetic Materials 631
17.12 Soft Magnetic Materials 635

References 641
Problems 641


W17.1 Details on Domain Structures
W17.2 Details on Size and Shape Effects
W17.3 Details on Magnetostriction
W17.4 Giant and Colossal Magnetoresistance
W17.5 Faraday and Kerr Effects
W17.6 Details on Dynamic Magnetic Effects
W17.7 Technologically Important Magnetic Materials
W17.8 Details on Permanent-Magnet Materials
W17.9 Details on Magnetic Recording Materials
W17.10 Details on Magneto-Optical Recording Materials
W17.11 Details on Fe Alloys and Electrical Steels
W17.12 Details on Materials for Read/Write Heads
W17.13 Details on Magnetostrictive Materials
W17.14 Dilute Magnetic Semiconductors

References 641
Problems

18 Optical Materials 645

18.1 Introduction 645
Propagation of Light 646
CONTENTS

18.2 Optical Fibers 646
Generation of Light 650
18.3 Lasers 650
18.4 Light-Emitting Diodes and Semiconductor Lasers 653
18.5 Ceramics for Lasers 657
18.6 Bandgap Engineering of Optical Materials 659
Recording of Light 662
18.7 Photography 662
18.8 Photoconductors and Xerography 666
18.9 Electro-optic Effect and Photorefractive Materials 668
References 674
Problems 675

W18.1 Optical Polarizers
W18.2 Faraday Rotation
W18.3 Theory of Optical Band Structure
W18.4 Damage
References
Problem

SECTION IV SURFACES, THIN FILMS, INTERFACES, AND
MULTILAYERS

19 Surfaces 679

19.1 Introduction 679
19.2 Ideal Surfaces 680
Real Surfaces 682
19.3 Relaxation 682
19.4 Reconstruction 685
19.5 Surface Defects 687
Electronic Properties of Surfaces 690
19.6 Work Function 690
19.7 Thermionic Emission 693
19.8 Field Emission 695
19.9 Photoemission 697
19.10 Surface States 698
Surface Modification 699
19.11 Anodization 699
19.12 Passivation 700
19.13 Surface Phonons 702
19.14 Surface Processes 705
Adhesion and Friction 707
19.15 Surface Plasmons 707
19.16 Dispersion Forces 708
19.17 Friction 710
References 713
Problems 713

W19.1 Surface States
W19.2 Surfactants
W19.3 Adsorption
W19.4 Desorption
W19.5 Surface Diffusion
W19.6 Catalysis
W19.7 Friction
Appendix W19A: Construction of the Surface Net
Appendix W19B: Fowler–Nordheim Formula
Appendix W19C: Photoemission Yields

20 Thin Films, Interfaces, and Multilayers 715

20.1 Introduction 715
Thin Films
20.2 Surface Tension 716
20.3 Thin-Film Fabrication 718
20.4 Morphology Maps 721
20.5 Langmuir–Blodgett Films 723
Interfaces 725
20.6 Grain Boundaries 726
20.7 Band Bending in Semiconductors 729
20.8 Schottky Barrier 732
20.9 Semiconductor–Heterostructure Superlattices 734
20.10 Quantum Dot 737
20.11 Si/a-SiO2 Interface 740
Multilayers 742
20.12 X-ray Mirrors 742
20.13 Hardness of Multilayers 743
20.14 Stoichiometric Optimization of Physical Parameters 744
References 746
Problems 747

W20.1 Strength and Toughness
W20.2 Critical Thickness
W20.3 Ionic Solutions
W20.4 Solid–Electrolyte Interface
W20.5 Multilayer Materials
W20.6 Second-Harmonic Generation in Phase-Matched Multilayers
W20.7 Organic Light-Emitting Diodes
W20.8 Quasiperiodic Nonlinear Optical Crystals
W20.9 Graphite Intercalated Compounds
SECTION V SYNTHESIS AND PROCESSING OF MATERIALS

21 Synthesis and Processing of Materials 751

21.1 Introduction 751

Issues in Synthesis and Processing 752

21.2 Thermodynamic and Chemical Effects 753
21.3 Kinetic Effects 757
21.4 Crystal Growth 762
21.5 Annealing 764

Synthesis and Processing of Semiconductors 767

21.6 Czochralski Growth of Single-Crystal Silicon 768
21.7 Thermal Oxidation of Silicon 771
21.8 Fabrication of Silicon Devices 775

Synthesis and Processing of Metals 778

21.9 Synthesis and Processing of Steels 779
21.10 Synthesis and Processing of Stainless Steels 785

Synthesis and Processing of Ceramics and Glasses 787

21.11 Powder Synthesis 788
21.12 Sol–Gel Synthesis 790

Synthesis and Processing of Polymers and Carbon Molecules 792

21.13 Polymerization 792
21.14 Catalysts in Polymer Synthesis 794
21.15 Synthesis of Carbon Nanotubes 796

References 798
Problems 799


W21.1 Synthesis and Processing Procedures
W21.2 Heteroepitaxial Growth
W21.3 Processing Using Ion Beams
W21.4 Float-Zone Purification of Single-Crystal Si
W21.5 Epitaxial Growth of Single-Crystal Si Layers via CVD
W21.6 Molecular-Beam Epitaxial Growth of GaAs
W21.7 Plasma-Enhanced CVD of Amorphous Semiconductors
W21.8 Fabrication of Si Devices
W21.9 Processing of Microelectromechanical Systems
W21.10 Synthesis and Processing of Steels
W21.11 Precipitation Hardening of Aluminum Alloys
W21.12 Synthesis of Metals via Rapid Solidification
W21.13 Surface Treatments for Metals
W21.14 Chemical Vapor Deposition of Diamond
W21.15 Synthesis of YBa2Cu3O7−x
W21.16 Synthesis of Si$_3$N$_4$
W21.17 Synthesis of SiC
W21.18 Synthesis of the Zeolite ZSM-5
W21.19 Synthesis of the Perovskite PLZT
W21.20 Synthesis of Glasses: Pilkington Process
W21.21 Synthesis of Polycarbonate
W21.22 Synthesis of Polystyrene
W21.23 Synthesis of Electro-active Polymers
W21.24 Spin Coating
W21.25 Microwave and Plasma Processing of Polymers

References

Problems

22 Characterization of Materials

W22.1 Introduction

Diffraction Techniques
W22.2 X-ray Diffraction
W22.3 Low-Energy Electron Diffraction
W22.4 Reflection High-Energy Electron Diffraction
W22.5 Neutron Scattering

Optical Spectroscopy
W22.6 Optical Spectroscopy in the Infrared, Visible, and Ultraviolet
W22.7 Ellipsometry
W22.8 Fourier Transform Infrared Spectroscopy
W22.9 Raman Spectroscopy
W22.10 Luminescence
W22.11 Nonlinear Optical Spectroscopy

Electron Microscopy
W22.12 Scanning-Electron Microscopy
W22.13 Transmission-Electron Microscopy
W22.14 High-Resolution Transmission-Electron Microscopy
W22.15 Low-Energy Electron Microscopy

Electron Spectroscopy and Ion Scattering
W22.16 Photoemission
W22.17 Low-Energy Electron Loss Spectroscopy
W22.18 Extended X-ray Absorption Fine Structure
W22.19 Auger Emission Spectroscopy
W22.20 Secondary-Ion Mass Spectrometry
W22.21 Rutherford Backscattering

Surface Microscopy
W22.22 Atomic-Force Microscopy
W22.23 Scanning-Tunneling Microscope
W22.24 Lateral-Force Microscope and Surface Force Apparatus

Transport Measurements
W22.25 Electrical Resistivity and Hall Effect
As science has become more interdisciplinary and impinges ever more heavily on technology, we have been led to the conclusion that there is a great need now for a textbook that emphasizes the physical and chemical origins of the properties of solids while at the same time focusing on the technologically important materials that are being developed and used by scientists and engineers. A panel of physicists, chemists, and materials scientists who participated in the NSF Undergraduate Curriculum Workshop in Materials in 1989, which addressed educational needs and opportunities in the area of materials research and technology, issued a report that indicated clearly the need for advanced textbooks in materials beyond the introductory level. Our textbook is meant to address this need.

This textbook is designed to serve courses that provide engineering and science majors with their first in-depth introduction to the properties and applications of a wide range of materials. This ordinarily occurs at the advanced undergraduate level but can also occur at the graduate level. The philosophy of our approach has been to define consistently the structure and properties of solids on the basis of the local chemical bonding and atomic order (or disorder!) present in the material. Our goal has been to bring the science of materials closer to technology than is done in most traditional textbooks on solid-state physics. We have stressed properties and their interpretation and have avoided the development of formalism for its own sake. We feel that the specialized mathematical techniques that can be applied to predict the properties of solids are better left for more advanced, graduate-level courses.

This textbook will be appropriate for use in the advanced materials courses given in engineering departments. Such courses are widely taught at the junior/senior level with such titles as “Principles of Materials Science & Engineering,” “Physical Electronics,” “Electronics of Materials,” and “Engineering Materials.” This textbook is also designed to be appropriate for use by physics and chemistry majors. We note that a course in materials chemistry is a relatively new one in most chemistry undergraduate curricula but that an introductory course in solid-state physics has long been standard in physics undergraduate curricula.

To gain the most benefit from courses based on this textbook, students should have had at least one year each of introductory physics, chemistry, and calculus, along with a course in modern physics or physical chemistry. For optimal use of the textbook it would be helpful if the students have had courses in thermodynamics, electricity and magnetism, and an introduction to quantum mechanics.

As the title indicates, the range of topics covered in this textbook is quite broad. The 21 chapters are divided into five sections. The range of topics covered is comprehensive, but not exhaustive. For example, topics not covered in detail due to lack of space include biomaterials, a field with a bright future, and composites, examples of which are discussed only within specific classes of materials. Much more material is presented
than can be covered in a one-semester course. Actual usage of the text in courses will be discussed after the proposed subject matter has been outlined.

Following an introduction, which emphasizes the importance of materials in modern science and technology, Section I, on the “Structure of Materials,” consists of four chapters on the structure of crystals, bonding in solids, diffraction and the reciprocal lattice, and order and disorder in solids.

Section II, on the “Physical Properties of Materials,” consists of six chapters on phonons; thermally activated processes, phase diagrams, and phase transitions; electrons in solids: electrical and thermal properties; optical properties; magnetic properties; and mechanical properties.

Section III, titled “Classes of Materials,” consists of eight chapters on semiconductors; metals and alloys; ceramics; polymers; dielectric and ferroelectric materials; superconductors; magnetic materials; and optical materials. In each chapter the distinctive properties of each class of materials are discussed using technologically-important examples from each class. In addition, the structure and key properties of selected materials are highlighted. In this way an indication of the wide spectrum of materials in each class is presented.

Section IV, titled “Surfaces, Thin Films, Interfaces, and Multilayers,” consists of two chapters covering these important topics. Here the effects of spatial discontinuities in the physical and chemical structure on the properties of materials are presented, both from the point of view of creating materials with new properties and also of minimizing the potential materials problems associated with surfaces and interfaces.

Section V, titled “Synthesis and Processing of Materials,” consists of a single chapter. Representative examples of how the structure and properties of materials are determined by the techniques used to synthesize them are presented. “Atomic engineering” is stressed. The tuning of structure and properties using postsynthesis processing is also illustrated.

Problem sets are presented at the end of each chapter and are used to emphasize the most important concepts introduced, as well as to present further examples of important materials. Illustrations are employed for the purpose of presenting crystal structures and key properties of materials. Tables are used to summarize and contrast the properties of related groups of materials. The units used throughout this textbook are SI units, except in cases where the use of electron volt, cm$^{-1}$, poise, etc., were felt to be too standard to ignore.

We have created a home page at www.wiley.com that provides a valuable supplement to the textbook by describing additional properties of materials, along with additional examples of current materials and their applications. Chapter W22 on our home page emphasizes the structural and chemical characterization of materials, as well as the characterization of their optical, electrical, and magnetic properties. As new materials and applications are developed, the home page will be regularly updated.

Since this text will likely be used most often in a one-semester course, we recommend that Chapters 1–4 on structure be covered in as much detail as needed, given the backgrounds of the students. A selection of chapters on the properties of materials (5–10) and on the classes of materials (11–18) of particular interest can then be covered. According to the tastes of the instructor and the needs of the students, some of the remaining chapters (surfaces; thin films, interfaces, and multilayers; synthesis and processing of materials) can be covered. For example, a course on engineering materials
could consist of the following: Chapters 1–4 on structure; Chapter 6 on thermally activated processes, etc.; Chapter 10 on mechanical properties; Chapter 12 on metals and alloys; Chapter 13 on ceramics; Chapter 14 on polymers; and Chapter 21 on synthesis and processing.

Physics majors usually take an introductory course in solid-state physics in their senior year. Therefore in such a course it will be necessary to start at “the beginning,” i.e., Chapter 1 on the structure of crystals. Students in MS&E or engineering departments who have already taken an introductory course on materials can quickly review (or skip) much of the basic material and focus on more advanced topics, beginning with Chapter 5 on phonons, if desired, or Chapter 7 on electrons in solids.

We owe a debt of gratitude to our colleagues at The City College and City University who, over the years, have shared with us their enthusiasm for and interest in the broad and fascinating subject of materials. They include R. R. Alfano, J. L. Birman, T. Boyer, F. Cadieu, H. Z. Cummins, H. Falk, A. Genack, M. E. Green, L. L. Isaacs, M. Lax, D. M. Lindsay (deceased), V. Petricevic, F. H. Pollak, S. R. Radel, M. P. Sarachik, D. Schmeltzer, S. Schwarz, J. Steiner, M. Tamargo, M. Tzolkevic, and N. Tzoar (deceased). Colleagues outside CUNY who have shared their knowledge with us include Z. L. Akkerman, R. Dessau, Efstathiadis, B. Gersten, Y. Goldstein, P. Jacoby, L. Ley, K. G. Lynn, D. Rahoi, and Z. Yin. Our thanks also go to our students and postdocs who have challenged us, both in our research and teaching, to refine our thinking about materials and their behavior.

Special thanks are due to Gregory Franklin who served as our editor at John Wiley & Sons for the bulk of the preparation of this textbook. His unflagging support of this effort and his patience are deeply appreciated. Thanks are also due to our current editor, George Telecki, who has helped us with sound advice to bring this project to a successful conclusion. We acknowledge with gratitude the skill of Angioline Loredo who supervised the production of both the textbook and supplementary Web-based material. We have appreciated the useful comments of all the anonymous reviewers of our textbook and also wish to thank all the authors who granted permission for us to use their artwork.

Finally, we gratefully acknowledge the constant support, encouragement, and patience of our wives, Harriet and Francoise, and our families during the years in which this textbook was prepared. Little did we (or they) know how long it would take to accomplish our goals.

JOEL I. GERSTEN
FREDERICK W. SMITH

New York City
LIST OF TABLES

1.1 Bravais lattices in three dimensions 10
1.2 Local atomic bonding units 16
1.3 Elements with HCP crystal structure 22
1.4 Periodic table with crystal structures and lattice constants 23
1.5 Elements with FCC crystal structure 24
1.6 Elements with BCC crystal structure 26
1.7 Crystals with CsCl crystal structure 27
1.8 Crystals with NaCl crystal structure 28
1.9 Elements with diamond crystal structure 29
1.10 Crystals with zincblende crystal structure 30
1.11 Periodic table with densities and atomic concentrations 33
2.1 Structures of covalently bonded elements 43
2.2 Classification of solids according to bonding 47
2.3 Radius ratios and crystal structures 50
2.4 Ionic radii 52
2.5 Radius ratios and crystal structures of alkali chlorides 52
2.6 Ionicities of some crystals 54
2.7 Periodic table of cohesive energies 56
2.8 Cohesive energies of some crystals 57
2.9 Periodic table of first and second ionization energies 59
2.10 Periodic table of electron affinities 61
2.11 Periodic table of electronegativities 62
2.12 Periodic table of atomic radii 63
2.13 Van der Waals radii 64
4.1 Crystallite sizes and types of structural order 87
4.2 Properties of vacancies in FCC metals 117
5.1 Molar specific heat 133
5.2 Debye temperatures 138
5.3 Thermal expansion coefficients and Gruneisen constants 143
5.4 Thermal conductivities 144
6.1 Periodic table of melting points and enthalpies of fusion 174
6.2 Test of Lindemann criterion 176
6.3 Melting points and cohesion data for crystals 179
6.4 Characteristics of solid-state structural phase transitions 180
7.1 Atomic numbers, valences, mass densities, electron densities, conductivities, and collision times of metals 189
7.2 Hall coefficients 191
7.3 Free-electron parameters 193
7.4 Percolation thresholds 221
8.1 The electromagnetic spectrum 232
8.2 Plasma energies 235
8.3 Ionic frequencies 241
8.4 Nonlinear optical coefficients at \( \lambda = 1.06 \) \( \mu \)m 249
8.5 Some third-order susceptibilities 250
8.6 Exciton parameters for several semiconductors 252
9.1 Ground states of 3d transition elements 268
9.2 Crystal field stabilization energies and spins for 3d ions 272
9.3 Ground states of 4f rare earth elements 275
9.4 Magnetic properties of ferro-, antiferro-, and ferrimagnets 288
9.5 1st and 2nd-order magnetocrystalline anisotropy coefficients 296
9.6 Crystals containing magnetic Fe ions 303
9.7 Magnetic susceptibilities for selected materials 308
10.1 Independent elastic constants for different Bravais lattices 319
10.2 Elastic properties of polycrystalline cubic metals 322
10.3 Elastic constants for various single crystals 323
10.4 Relationships between elastic moduli of isotropic solids 325
10.5 Elastic wave velocities in cubic crystals 329
10.6 Mechanical properties of selected materials 338
10.7 Slip planes and directions 346
10.8 Fracture toughness of various materials 350
11.1 Energy gaps and electron concentrations of selected semiconductors 358
11.2 Properties of electrons and holes 371
11.3 Comparison of Bohr theory and dopant impurity model 376
11.4 Dopant activation energies 377
11.5 Properties of electrons in solids of reduced dimensionality 384
11.6 Electron and hole mobilities and conductivities 390
11.7 Properties of group IV semiconductors 406
11.8 Effective masses and mobilities of charge carriers 407
11.9 Properties of group III–V, II–VI, and IV–VI semiconductors 411
11.10 Interfaces between semiconductors and other materials 435
12.1 Properties of \( sp \)-bonded metals 448
12.2 Selected properties of the rare earth metals 453
12.3 Chemical composition of superalloys 461
13.1 Properties of ceramic materials: crystal structure, melting temperature, Young’s modulus, thermal expansion coefficient, thermal conductivity and Knoop hardness 466
13.2 Madelung constant for binary ionic solids 471
13.3 Melting temperatures of refractory materials 472
13.4 Melting temperatures of glass-forming materials 482
13.5 Composition of some common commercial glasses 487
14.1 Crystal structure parameters for polymers 499
14.2 Mechanical properties of polymers 502
14.3 Thermal properties of polymers 511
14.4 Glass-transition and melting temperatures for polymers 513
15.1 Optical phonon energies and dielectric constants 530
15.2 Dielectric strengths 532
15.3 Polarization properties of ferroelectrics 536
<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>15.4</td>
<td>Barrier heights and conductivities for beta aluminas</td>
<td>546</td>
</tr>
<tr>
<td>16.1</td>
<td>Periodic table of superconducting $T_c$ and $H_{c0}$</td>
<td>557</td>
</tr>
<tr>
<td>16.2</td>
<td>Superconducting energy gap ratio $2\varepsilon(0)/k_B T_c$</td>
<td>563</td>
</tr>
<tr>
<td>16.3</td>
<td>Predictions of BCS theory in weak-coupling limit</td>
<td>578</td>
</tr>
<tr>
<td>16.4</td>
<td>Properties $\lambda(0 \text{ K})$, $\xi(0 \text{ K})$, $\kappa(T_c)$ of various superconductors</td>
<td>583</td>
</tr>
<tr>
<td>16.5</td>
<td>Families of cuprate superconductors</td>
<td>585</td>
</tr>
<tr>
<td>16.6</td>
<td>Upper critical fields for various high-field superconductors</td>
<td>592</td>
</tr>
<tr>
<td>17.1</td>
<td>Magnetostrictions of ferromagnets and ferrimagnets</td>
<td>626</td>
</tr>
<tr>
<td>17.2</td>
<td>Properties of permanent-magnet materials</td>
<td>632</td>
</tr>
<tr>
<td>17.3</td>
<td>Magnetic properties of Fe, Fe alloys, and electrical steels</td>
<td>637</td>
</tr>
<tr>
<td>17.4</td>
<td>Magnetic materials with giant magnetostrictions</td>
<td>638</td>
</tr>
<tr>
<td>17.5</td>
<td>Magnetic properties of ferrimagnetic garnets</td>
<td>640</td>
</tr>
<tr>
<td>18.1</td>
<td>Lattice constants, band gap energies, conduction band masses, light- and heavy-hole band masses, static relative permittivities, high-frequency relative permittivities, thermal conductivities, coefficients of linear thermal expansion, phonon frequencies, and band-offset parameters for III–V semiconductors</td>
<td>656</td>
</tr>
<tr>
<td>18.2</td>
<td>Triboelectric series</td>
<td>668</td>
</tr>
<tr>
<td>18.3</td>
<td>Electro-optic tensor components</td>
<td>671</td>
</tr>
<tr>
<td>19.1</td>
<td>Surface nets and primitive lattice vectors</td>
<td>682</td>
</tr>
<tr>
<td>19.2</td>
<td>Work functions and first ionization energies</td>
<td>692</td>
</tr>
<tr>
<td>19.3</td>
<td>Coefficients of static friction</td>
<td>712</td>
</tr>
<tr>
<td>20.1</td>
<td>Surface tensions</td>
<td>717</td>
</tr>
<tr>
<td>20.2</td>
<td>Typical quantum-dot systems</td>
<td>740</td>
</tr>
<tr>
<td>21.1</td>
<td>International Technology Road Map for Semiconductors</td>
<td>776</td>
</tr>
<tr>
<td>21.2</td>
<td>Important phases of Fe, Fe compounds and alloys, and their multicomponent mixtures</td>
<td>781</td>
</tr>
<tr>
<td>21.3</td>
<td>Compositions of typical austenitic stainless steels</td>
<td>786</td>
</tr>
<tr>
<td>21.4</td>
<td>Physical properties of fullerene</td>
<td>798</td>
</tr>
</tbody>
</table>