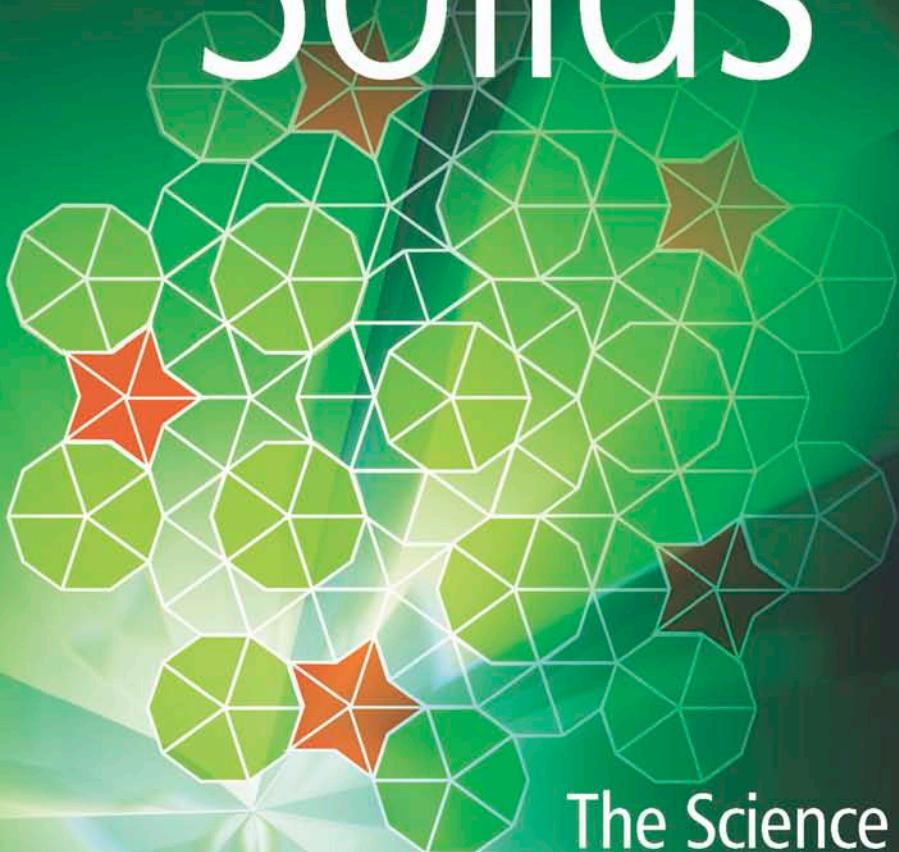


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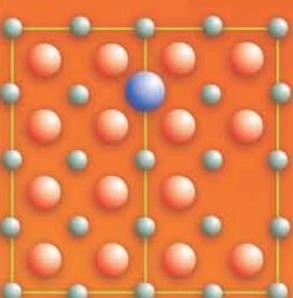
Second Edition

Understanding Solids



The Science of Materials

 WILEY



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Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
IA	H	IIA	IIIB	IVB	VB	VIB	VIIIB				IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIII
1	1 H 1s ¹																2 He 1s ²	
2	3 Li 2s ¹	4 Be 2s ²																
3	11 Na 3s ¹	12 Mg 3s ²																
4	19 K 4s ¹	20 Ca 4s ²	21 Sc 4s ² 3d ¹	22 Ti 4s ² 3d ²	23 V 4s ² 3d ³	24 Cr 4s ¹ 3d ⁵	25 Mn 4s ³ d ⁵	26 Fe 4s ² 3d ⁶	27 Co 4s ² 3d ⁷	28 Ni 4s ² 3d ⁸	29 Cu 4s ¹ 3d ¹⁰	30 Zn 4s ² 3d ¹⁰	31 Ga 4s ² 4p ¹	32 Ge 4s ² 4p ²	33 As 4s ² 4p ³	34 Se 4s ² 4p ⁴	35 Br 4s ² 4p ⁵	36 Kr 4s ² 4p ⁶
5	37 Rb 5s ¹	38 Sr 5s ²	39 Y 5s ² 4d ¹	40 Zr 5s ² 4d ²	41 Nb 5s ⁴ d ³	42 Mo 5s ⁴ d ⁵	43 Tc 5s ⁴ d ⁶	44 Ru 5s ⁴ d ⁷	45 Rh 5s ⁴ d ⁸	46 Pd 5s ⁴ d ⁹	47 Ag 5s ⁴ d ¹⁰	48 Cd 5s ⁵ p ¹	49 In 5s ⁵ p ²	50 Sn 5s ⁵ p ³	51 Sb 5s ⁵ p ⁴	52 Te 5s ⁵ p ⁵	53 I 5s ⁵ p ⁶	54 Xe 5s ⁵ p ⁶
6	55 Cs 6s ¹	56 Ba 6s ²	71 Lu 6s ² 5d ¹	72 Hf 6s ² 5d ²	73 Ta 6s ² 5d ³	74 W 6s ² 5d ⁴	75 Re 6s ² 5d ⁵	76 Os 6s ² 5d ⁶	77 Ir 6s ² 5d ⁷	78 Pt 6s ¹ 5d ¹⁰	79 Au 6s ² 5d ¹⁰	80 Hg 6s ² 6p ¹	81 Tl 6s ² 6p ²	82 Pb 6s ² 6p ³	83 Bi 6s ² 6p ⁴	84 Po 6s ² 6p ⁵	85 At 6s ² 6p ⁶	86 Rn 6s ² 6p ⁶
7	87 Fr 7s ¹	88 Ra 7s ²	103 Lr 7s ² 6d ¹	104 Rf 7s ² 6d ²	105 Db 7s ² 6d ³	106 Sg 7s ² 6d ⁴	107 Bh 7s ² 6d ⁵	108 Hs 7s ² 6d ⁶	109 Mt 7s ² 6d ⁷									
			57 La 6s ² 5d ¹	58 Ce 6s ² 4f ²	59 Pr 6s ² 4f ³	60 Nd 6s ² 4f ⁴	61 Pm 6s ² 4f ⁵	62 Sm 6s ² 4f ⁶	63 Eu 6s ² 4f ⁷	64 Gd 6s ² 5d ¹ 4f ¹	65 Tb 6s ² 4f ⁹	66 Dy 6s ² 4f ¹⁰	67 Ho 6s ² 4f ¹¹	68 Er 6s ² 4f ¹²	69 Tm 6s ² 4f ¹³	70 Yb 6s ² 4f ¹⁴		
			89 Ac 7s ² 6d ¹	90 Th 7s ² 6d ²	91 Pa 7s ² 6d ³	92 U 7s ² 6d ⁴	93 Np 7s ² 6d ⁵	94 Pu 7s ² 5f ⁰	95 Am 7s ² 5f ¹	96 Cm 7s ² 5f ²	97 Bk 7s ² 5f ³	98 Cf 7s ² 5f ¹⁰	99 Es 7s ² 5f ¹¹	100 Fm 7s ² 5f ¹²	101 Md 7s ² 5f ¹³	102 No 7s ² 5f ¹⁴		

Understanding Solids

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The Science of Materials

2nd edition

Richard J.D. Tilley
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For Anne

Contents

Preface to the Second Edition	xvii
Preface to the First Edition	xix
PART 1 STRUCTURES AND MICROSTRUCTURES	1
1 The electron structure of atoms	3
1.1 The hydrogen atom	3
1.1.1 The quantum mechanical description	3
1.1.2 The energy of the electron	4
1.1.3 Electron orbitals	5
1.1.4 Orbital shapes	5
1.2 Many-electron atoms	7
1.2.1 The orbital approximation	7
1.2.2 Electron spin and electron configuration	7
1.2.3 The periodic table	9
1.3 Atomic energy levels	11
1.3.1 Spectra and energy levels	11
1.3.2 Terms and term symbols	11
1.3.3 Levels	13
1.3.4 Electronic energy level calculations	14
Further reading	15
Problems and exercises	16
2 Chemical bonding	19
2.1 Ionic bonding	19
2.1.1 Ions	19
2.1.2 Ionic size and shape	20
2.1.3 Lattice energies	21
2.1.4 Atomistic simulation	23
2.2 Covalent bonding	24
2.2.1 Valence bond theory	24
2.2.2 Molecular orbital theory	30
2.3 Metallic bonding and energy bands	35
2.3.1 Molecular orbitals and energy bands	36
2.3.2 The free electron gas	37
2.3.3 Energy bands	40

2.3.4 Properties of metals	41
2.3.5 Bands in ionic and covalent solids	43
2.3.6 Computation of properties	44
Further reading	45
Problems and exercises	46
3 States of aggregation	49
3.1 Weak chemical bonds	49
3.2 Macrostructures, microstructures and nanostructures	52
3.2.1 Structures and scale	52
3.2.2 Crystalline solids	52
3.2.3 Quasicrystals	53
3.2.4 Non-crystalline solids	54
3.2.5 Partly crystalline solids	55
3.2.6 Nanoparticles and nanostructures	55
3.3 The development of microstructures	57
3.3.1 Solidification	58
3.3.2 Processing	58
3.4 Point defects	60
3.4.1 Point defects in crystals of elements	60
3.4.2 Solid solutions	61
3.4.3 Schottky defects	62
3.4.4 Frenkel defects	63
3.4.5 Non-stoichiometric compounds	64
3.4.6 Point defect notation	66
3.5 Linear, planar and volume defects	68
3.5.1 Edge dislocations	68
3.5.2 Screw dislocations	69
3.5.3 Partial and mixed dislocations	69
3.5.4 Planar defects	69
3.5.5 Volume defects: precipitates	70
Further reading	73
Problems and exercises	73
4 Phase diagrams	77
4.1 Phases and phase diagrams	77
4.1.1 One-component (unary) systems	77
4.1.2 The phase rule for one-component (unary) systems	79
4.2 Binary phase diagrams	80
4.2.1 Two-component (binary) systems	80
4.2.2 The phase rule for two-component (binary) systems	81
4.2.3 Simple binary diagrams: nickel–copper as an example	81
4.2.4 Binary systems containing a eutectic point: tin–lead as an example	83
4.2.5 Intermediate phases and melting	87
4.3 The iron–carbon system near to iron	88
4.3.1 The iron–carbon phase diagram	88
4.3.2 Steels and cast irons	89
4.3.3 Invariant points	89
4.4 Ternary systems	90

4.5 Calculation of phase diagrams: CALPHAD	93
Further reading	94
Problems and exercises	94
5 Crystallography and crystal structures	101
5.1 Crystallography	101
5.1.1 Crystal lattices	101
5.1.2 Crystal systems and crystal structures	102
5.1.3 Symmetry and crystal classes	104
5.1.4 Crystal planes and Miller indices	106
5.1.5 Hexagonal crystals and Miller-Bravais indices	109
5.1.6 Directions	110
5.1.7 Crystal geometry and the reciprocal lattice	112
5.2 The determination of crystal structures	114
5.2.1 Single crystal X-ray diffraction	114
5.2.2 Powder X-ray diffraction and crystal identification	115
5.2.3 Neutron diffraction	118
5.2.4 Electron diffraction	118
5.3 Crystal structures	118
5.3.1 Unit cells, atomic coordinates and nomenclature	118
5.3.2 The density of a crystal	119
5.3.3 The cubic close-packed (A1) structure	121
5.3.4 The body-centred cubic (A2) structure	121
5.3.5 The hexagonal (A3) structure	122
5.3.6 The diamond (A4) structure	122
5.3.7 The graphite (A9) structure	123
5.3.8 The halite (rock salt, sodium chloride, B1) structure	123
5.3.9 The spinel (H_1) structure	125
5.4 Structural relationships	126
5.4.1 Sphere packing	126
5.4.2 Ionic structures in terms of anion packing	128
5.4.3 Polyhedral representations	129
Further reading	131
Problems and exercises	131
PART 2 CLASSES OF MATERIALS	137
6 Metals, ceramics, polymers and composites	139
6.1 Metals	139
6.1.1 The crystal structures of pure metals	140
6.1.2 Metallic radii	141
6.1.3 Alloy solid solutions	142
6.1.4 Metallic glasses	145
6.1.5 The principal properties of metals	146
6.2 Ceramics	147
6.2.1 Bonding and structure of silicate ceramics	147
6.2.2 Some non-silicate ceramics	149
6.2.3 The preparation and processing of ceramics	152
6.2.4 The principal properties of ceramics	154

6.3	Silicate glasses	154
6.3.1	Bonding and structure of silicate glasses	155
6.3.2	Glass deformation	157
6.3.3	Strengthened glass	159
6.3.4	Glass-ceramics	160
6.4	Polymers	161
6.4.1	Polymer formation	162
6.4.2	Microstructures of polymers	165
6.4.3	Production of polymers	170
6.4.4	Elastomers	173
6.4.5	The principal properties of polymers	175
6.5	Composite materials	177
6.5.1	Fibre-reinforced plastics	177
6.5.2	Metal-matrix composites	177
6.5.3	Ceramic-matrix composites	178
6.5.4	Cement and concrete	178
	Further reading	181
	Problems and exercises	182
PART 3 REACTIONS AND TRANSFORMATIONS		189
7	Diffusion and ionic conductivity	191
7.1	Self-diffusion, tracer diffusion and tracer impurity diffusion	191
7.2	Non-steady-state diffusion	194
7.3	Steady-state diffusion	195
7.4	Temperature variation of diffusion coefficient	195
7.5	The effect of impurities	196
7.6	Random walk diffusion	197
7.7	Diffusion in solids	198
7.8	Self-diffusion in one dimension	199
7.9	Self-diffusion in crystals	201
7.10	The Arrhenius equation and point defects	202
7.11	Correlation factors for self-diffusion	204
7.12	Ionic conductivity	205
7.12.1	Ionic conductivity in solids	205
7.12.2	The relationship between ionic conductivity and diffusion coefficient	208
	Further reading	209
	Problems and exercises	209
8	Phase transformations and reactions	213
8.1	Sintering	213
8.1.1	Sintering and reaction	213
8.1.2	The driving force for sintering	215
8.1.3	The kinetics of neck growth	216
8.2	First-order and second-order phase transitions	216
8.2.1	First-order phase transitions	217
8.2.2	Second-order transitions	217

8.3	Displacive and reconstructive transitions	218
8.3.1	Displacive transitions	218
8.3.2	Reconstructive transitions	219
8.4	Order-disorder transitions	221
8.4.1	Positional ordering	221
8.4.2	Orientational ordering	222
8.5	Martensitic transformations	223
8.5.1	The austenite-martensite transition	223
8.5.2	Martensitic transformations in zirconia	226
8.5.3	Martensitic transitions in Ni-Ti alloys	227
8.5.4	Shape-memory alloys	228
8.6	Phase diagrams and microstructures	230
8.6.1	Equilibrium solidification of simple binary alloys	230
8.6.2	Non-equilibrium solidification and coring	230
8.6.3	Solidification in systems containing a eutectic point	231
8.6.4	Equilibrium heat treatment of steel in the Fe-C phase diagram	233
8.7	High-temperature oxidation of metals	236
8.7.1	Direct corrosion	236
8.7.2	The rate of oxidation	236
8.7.3	Oxide film microstructure	237
8.7.4	Film growth via diffusion	238
8.7.5	Alloys	239
8.8	Solid-state reactions	240
8.8.1	Spinel formation	240
8.8.2	The kinetics of spinel formation	241
	Further reading	242
	Problems and exercises	242

9 Oxidation and reduction 247

9.1	Galvanic cells	247
9.1.1	Cell basics	247
9.1.2	Standard electrode potentials	249
9.1.3	Cell potential and Gibbs energy	250
9.1.4	Concentration dependence	251
9.2	Chemical analysis using galvanic cells	251
9.2.1	pH meters	251
9.2.2	Ion selective electrodes	253
9.2.3	Oxygen sensors	254
9.3	Batteries	255
9.3.1	'Dry' and alkaline primary batteries	255
9.3.2	Lithium-ion primary batteries	256
9.3.3	The lead-acid secondary battery	257
9.3.4	Lithium-ion secondary batteries	257
9.3.5	Lithium-air batteries	259
9.3.6	Fuel cells	260
9.4	Corrosion	262
9.4.1	The reaction of metals with water and aqueous acids	262
9.4.2	Dissimilar metal corrosion	264
9.4.3	Single metal electrochemical corrosion	265
9.5	Electrolysis	266
9.5.1	Electrolytic cells	267
9.5.2	Electroplating	267

9.5.3	The amount of product produced during electrolysis	268
9.5.4	The electrolytic preparation of titanium by the <i>FFC Cambridge Process</i>	269
9.6	Pourbaix diagrams	270
9.6.1	Passivation, corrosion and leaching	270
9.6.2	The stability field of water	270
9.6.3	Pourbaix diagram for a metal showing two valence states, M^{2+} and M^{3+}	271
9.6.4	Pourbaix diagram displaying tendency for corrosion	273
	Further reading	274
	Problems and exercises	275

PART 4 PHYSICAL PROPERTIES 279

10	Mechanical properties of solids	281
10.1	Strength and hardness	281
10.1.1	Strength	281
10.1.2	Stress and strain	282
10.1.3	Stress–strain curves	283
10.1.4	Toughness and stiffness	286
10.1.5	Superelasticity	286
10.1.6	Hardness	287
10.2	Elastic moduli	289
10.2.1	Young’s modulus (the modulus of elasticity) (E or Y)	289
10.2.2	Poisson’s ratio (ν)	291
10.2.3	The longitudinal or axial modulus (L or M)	292
10.2.4	The shear modulus or modulus of rigidity (G or μ)	292
10.2.5	The bulk modulus, K or B	293
10.2.6	The Lamé modulus (λ)	293
10.2.7	Relationships between the elastic moduli	293
10.2.8	Ultrasonic waves in elastic solids	293
10.3	Deformation and fracture	295
10.3.1	Brittle fracture	295
10.3.2	Plastic deformation of metals	298
10.3.3	Dislocation movement and plastic deformation	298
10.3.4	Brittle and ductile materials	301
10.3.5	Plastic deformation of polymers	302
10.3.6	Fracture following plastic deformation	302
10.3.7	Strengthening	304
10.3.8	Computation of deformation and fracture	306
10.4	Time-dependent properties	307
10.4.1	Fatigue	307
10.4.2	Creep	308
10.5	Nanoscale properties	312
10.5.1	Solid lubricants	312
10.5.2	Auxetic materials	313
10.5.3	Thin films and nanowires	315
10.6	Composite materials	317
10.6.1	Young’s modulus of large particle composites	317
10.6.2	Young’s modulus of fibre-reinforced composites	318
10.6.3	Young’s modulus of a two-phase system	319
	Further reading	320
	Problems and exercises	321

11 Insulating solids	327
11.1 Dielectrics	327
11.1.1 Relative permittivity and polarisation	327
11.1.2 Polarisability	329
11.1.3 Polarisability and relative permittivity	330
11.1.4 The frequency dependence of polarisability and relative permittivity	331
11.1.5 The relative permittivity of crystals	332
11.2 Piezoelectrics, pyroelectrics and ferroelectrics	333
11.2.1 The piezoelectric and pyroelectric effects	333
11.2.2 Crystal symmetry and the piezoelectric and pyroelectric effects	335
11.2.3 Piezoelectric mechanisms	336
11.2.4 Quartz oscillators	337
11.2.5 Piezoelectric polymers	338
11.3 Ferroelectrics	340
11.3.1 Ferroelectric crystals	340
11.3.2 Hysteresis and domain growth in ferroelectric crystals	341
11.3.3 Antiferroelectrics	344
11.3.4 The temperature dependence of ferroelectricity and antiferroelectricity	344
11.3.5 Ferroelectricity due to hydrogen bonds	345
11.3.6 Ferroelectricity due to polar groups	347
11.3.7 Ferroelectricity due to medium-sized transition-metal cations	348
11.3.8 Poling and polycrystalline ferroelectric solids	349
11.3.9 Doping and modification of properties	349
11.3.10 Relaxor ferroelectrics	351
11.3.11 Ferroelectric nanoparticles, thin films and superlattices	352
11.3.12 Flexoelectricity in ferroelectrics	353
Further reading	354
Problems and exercises	355
12 Magnetic solids	361
12.1 Magnetic materials	361
12.1.1 Characterisation of magnetic materials	361
12.1.2 Magnetic dipoles and magnetic flux	362
12.1.3 Atomic magnetism	363
12.1.4 Overview of magnetic materials	365
12.2 Paramagnetic materials	368
12.2.1 The magnetic moment of paramagnetic atoms and ions	368
12.2.2 High and low spin: crystal field effects	369
12.2.3 Temperature dependence of paramagnetic susceptibility	371
12.2.4 Pauli paramagnetism	373
12.3 Ferromagnetic materials	374
12.3.1 Ferromagnetism	374
12.3.2 Exchange energy	376
12.3.3 Domains	378
12.3.4 Hysteresis	380
12.3.5 Hard and soft magnetic materials	380
12.4 Antiferromagnetic materials and superexchange	381
12.5 Ferrimagnetic materials	382
12.5.1 Cubic spinel ferrites	382
12.5.2 Garnet structure ferrites	383

12.5.3 Hexagonal ferrites	383
12.5.4 Double exchange	384
12.6 Nanostructures	385
12.6.1 Small particles and data recording	385
12.6.2 Superparamagnetism and thin films	386
12.6.3 Superlattices	386
12.6.4 Photoinduced magnetism	387
12.7 Magnetic defects	389
12.7.1 Magnetic defects in semiconductors	389
12.7.2 Charge and spin states in cobaltites and manganites	390
Further reading	393
Problems and exercises	393
13 Electronic conductivity in solids	399
13.1 Metals	399
13.1.1 Metals, semiconductors and insulators	399
13.1.2 Electron drift in an electric field	401
13.1.3 Electronic conductivity	402
13.1.4 Resistivity	404
13.2 Semiconductors	405
13.2.1 Intrinsic semiconductors	405
13.2.2 Band gap measurement	407
13.2.3 Extrinsic semiconductors	408
13.2.4 Carrier concentrations in extrinsic semiconductors	409
13.2.5 Characterisation	411
13.2.6 The p-n junction diode	413
13.3 Metal-insulator transitions	416
13.3.1 Metals and insulators	416
13.3.2 Electron-electron repulsion	417
13.3.3 Modification of insulators	418
13.3.4 Transparent conducting oxides	419
13.4 Conducting polymers	420
13.5 Nanostructures and quantum confinement of electrons	423
13.5.1 Quantum wells	424
13.5.2 Quantum wires and quantum dots	425
13.6 Superconductivity	426
13.6.1 Superconductors	426
13.6.2 The effect of magnetic fields	427
13.6.3 The effect of current	428
13.6.4 The nature of superconductivity	428
13.6.5 Josephson junctions	430
13.6.6 Cuprate high-temperature superconductors	430
Further reading	438
Problems and exercises	438
14 Optical aspects of solids	445
14.1 Light	445
14.1.1 Light waves	445
14.1.2 Photons	447
14.2 Sources of light	449

14.2.1	Incandescence	449
14.2.2	Luminescence and phosphors	450
14.2.3	Light-emitting diodes (LEDs)	453
14.2.4	Solid-state lasers	454
14.3	Colour and appearance	460
14.3.1	Luminous solids	460
14.3.2	Non-luminous solids	460
14.3.3	Attenuation	461
14.4	Refraction and dispersion	462
14.4.1	Refraction	462
14.4.2	Refractive index and structure	464
14.4.3	The refractive index of metals and semiconductors	465
14.4.4	Dispersion	465
14.5	Reflection	466
14.5.1	Reflection from a surface	466
14.5.2	Reflection from a single thin film	467
14.5.3	The reflectivity of a single thin film in air	469
14.5.4	The colour of a single thin film in air	469
14.5.5	The colour of a single thin film on a substrate	470
14.5.6	Low-reflectivity (antireflection) and high-reflectivity coatings	471
14.5.7	Multiple thin films and dielectric mirrors	471
14.6	Scattering	472
14.6.1	Rayleigh scattering	472
14.6.2	Mie scattering	475
14.7	Diffraction	475
14.7.1	Diffraction by an aperture	475
14.7.2	Diffraction gratings	476
14.7.3	Diffraction from crystal-like structures	477
14.7.4	Photonic crystals	478
14.8	Fibre optics	479
14.8.1	Optical communications	479
14.8.2	Attenuation in glass fibres	479
14.8.3	Dispersion and optical fibre design	480
14.8.4	Optical amplification	482
14.9	Energy conversion	483
14.9.1	Photoconductivity and photovoltaic solar cells	483
14.9.2	Dye sensitized solar cells	485
14.10	Nanostructures	486
14.10.1	The optical properties of quantum wells	486
14.10.2	The optical properties of nanoparticles	487
Further reading		489
Problems and exercises		489

15 Thermal properties 495

15.1	Heat capacity	495
15.1.1	The heat capacity of a solid	495
15.1.2	Classical theory of heat capacity	496
15.1.3	Quantum theory of heat capacity	496
15.1.4	Heat capacity at phase transitions	497
15.2	Thermal conductivity	498
15.2.1	Heat transfer	498
15.2.2	Thermal conductivity of solids	498

15.2.3	Thermal conductivity and microstructure	500
15.3	Expansion and contraction	501
15.3.1	Thermal expansion	501
15.3.2	Thermal expansion and interatomic potentials	502
15.3.3	Thermal contraction	503
15.3.4	Zero thermal contraction materials	505
15.4	Thermoelectric effects	506
15.4.1	Thermoelectric coefficients	506
15.4.2	Thermoelectric effects and charge carriers	508
15.4.3	The Seebeck coefficient of solids containing point defect populations	509
15.4.4	Thermocouples, power generation and refrigeration	509
15.5	The magnetocaloric effect	512
15.5.1	The magnetocaloric effect and adiabatic cooling	512
15.5.2	The giant magnetocaloric effect	513
	Further reading	514
	Problems and exercises	514
PART 5 NUCLEAR PROPERTIES OF SOLIDS		517
16	Radioactivity and nuclear reactions	519
16.1	Radioactivity	519
16.1.1	Naturally occurring radioactive elements	519
16.1.2	Isotopes and nuclides	520
16.1.3	Nuclear equations	520
16.1.4	Radioactive series	521
16.1.5	Nuclear stability	523
16.2	Artificial radioactive atoms	524
16.2.1	Transuranic elements	524
16.2.2	Artificial radioactivity in light elements	527
16.3	Nuclear decay	527
16.3.1	The rate of nuclear decay	527
16.3.2	Radioactive dating	529
16.4	Nuclear energy	531
16.4.1	The binding energy of nuclides	531
16.4.2	Nuclear fission	532
16.4.3	Thermal reactors for power generation	533
16.4.4	Fuel for space exploration	535
16.4.5	Fast breeder reactors	535
16.4.6	Fusion	535
16.4.7	Solar cycles	536
16.5	Nuclear waste	536
16.5.1	Nuclear accidents	537
16.5.2	The storage of nuclear waste	537
	Further reading	538
	Problems and exercises	539
Subject Index		543

Preface to the Second Edition

In this edition the structure of the First Edition has been retained. However, in the intervening years an enormous number of new experimental and theoretical studies have appeared in the literature, and although this is an introductory text, many of these new studies merit reporting. The additions are spread throughout the text, but can be roughly divided into four groups. The first area is computational science and engineering. Computer simulations of the behaviour of solids, from the engineering of large-scale structures using finite element analysis, via atomistic simulation and molecular dynamics, used to study features such as elastic behaviour and dislocation movement, through to the calculation of the electronic properties of solids via density functional theory, are used routinely in almost all disciplines that are related to the subject matter of this book. The computer calculation of phase diagrams (CALPHAD) also comes into this category. An indication of the principles underlying these programmes of work is given to underpin the computational “black boxes” available (Chapters 1, 2, 4 and 10).

Another area of change is that concerned with nanoscale properties. Here, not only is the primary literature growing rapidly but there are a rapidly increasing number of specialised books that deal with the subject. Some of the properties that are affected by small scales are described, including the magnetic and ferroelectric properties of thin films and superlattices (Chapters 11 and 12) and nanoparticle colours (Chapter 14).

Point defects are key components for the manipulation of the physical properties of solids, and this area has been supplemented. The universally used

Kroger-Vink notation for point defects has been defined (Chapter 3). The interplay between defect populations and ionic conductivity (Chapter 7), relaxor ferroelectrics (Chapter 11), the electronic and magnetic properties of cobaltites and manganites, including colossal magnetoresistance (Chapter 12, 13), cuprate superconductors (Chapter 13) and thermoelectric properties (Chapter 15) are described.

New text has also been added to cover a number of important crystallographically related topics. These include quasicrystals (Chapter 3), phase transformations including first- and second-order transitions, displacive versus reconstructive transitions and order-disorder transitions, and martensitic transitions (Chapter 9), and coverage of crystal symmetry with respect to piezoelectricity (Chapter 11).

Other new topics include lithium-air batteries (Chapter 8), increased discussion of elastic moduli and their measurement using ultrasonic waves (Chapter 10), the newly appreciated physical property of flexoelectricity (Chapter 11), crystal field effects, the magnetic properties of garnets and photoinduced magnetism (Chapter 12), dye-sensitized solar cells (Chapter 14), zero thermal expanding solids (Chapter 15), increased discussion of nuclear stability and radioisotope dating (Chapter 16).

The text on all these topics is necessarily compact, but can be supplemented by reference to extensive additional sources listed in the Further Reading sections.

Because of this expansion of material, of necessity some sections of the original have had to be excised. For the same reason, much of the supplementary information in the first edition has been

removed or incorporated into the relevant chapters. In making these changes, all the material has been rewritten and rearranged to the extent that no single page of this edition is identical to any in the first edition. In addition, all figures have been redrawn in colour. These, together with the solutions to the Introductory Questions and Problems and Exercises, are to be found on a companion web site (<http://www.wiley.com/go/tilleysolids2e>).

It is a pleasure to acknowledge the help from the staff at John Wiley, including Rebecca Stubbs, Emma Strickland and Sarah Tilley, all of whom

were enthusiastic about this project and fielded my many queries efficiently. The staff of the Trevithick library in Cardiff University provided, as always, help in tracking down obscure references. Professor F.S. Stone and Dr D.F. Klemperer were generous in their encouragement. Finally I must acknowledge my wife Anne, who has continually supported and helped in more ways than it is possible to record.

R.J.D. Tilley
August 2012

Preface to the First Edition

This book originated in lectures to undergraduate students in materials science, which were later extended to geology, physics and engineering students. The subject matter is concerned with the structures and properties of solids. The material is presented with a science bias, and is aimed not only at students taking traditional materials science and engineering courses, but also courses in the rapidly expanding fields of materials chemistry and physics. The coverage aims to be complementary to established books in materials science and engineering. The level is designed to be introductory in nature, and as far as is practical, the book is self-contained. The chapters are provided with questions designed to reinforce the concepts presented. These are in two parts. A multiple choice ‘Quick Quiz’ is designed to be tackled rapidly, and aims to uncover weaknesses in a student’s grasp of the fundamental concepts described. The ‘Calculations and Questions’ are more traditional, containing numerical examples to test the understanding of formulae, and derivations that are not carried out in the main body of the text. Many chapters contain one or more appendices that bear directly upon the material, but which would disrupt the flow of the subject matter if included within the chapter itself. These are meant to provide more depth than is possible otherwise. Further Reading allows students to take matters a little further. With only one exception, the references are to printed information. In general, it would be expected that a student would initially turn to the Internet for information. Sources here are rapidly located and this avenue of exploration has been left to the student.

The subject matter is divided into five sections. Part 1 covers the building blocks of solids. Here the topics centre upon atoms and bonding, and the patterns of structure that result. In this section, the important concepts of microstructure and macrostructure are developed, leading naturally to an understanding of why nanostructures possess unique properties. Defects that are of importance are also described here. Part 2 is concerned with the traditional triumvirate of metals, ceramics and polymers, together with a brief introduction to composite materials. The subject is condensed into a single chapter. It provides an overview of a comparative nature, focused upon giving a broad appreciation of why the fundamental groups of materials appear to differ so much, and laying the foundations for why some, such as ceramic superconductors, seem to behave so differently from their congeners. Part 3 has a more chemical bias, and describes reactions and transformations. The principles of diffusion are outlined in Chapter 7; electrochemical ideas, which lead naturally to batteries, corrosion and electroplating, are described in Chapter 8. Solid-state transformations, which impinge upon areas as diverse as shape memory alloys, semiconductor doping and sintering, are introduced in Chapter 9. Part 4 is a description of the physical properties of solids, and complements the chemical aspects detailed in Part 3. The topics covered are those of importance to both science and technology, mechanical, Chapter 10, insulators, Chapter 11, magnetic, Chapter 12, electronic, Chapter 13, optical, Chapter 14, and thermal, Chapter 15. Part 5 is concerned with radioactivity. This topic is of enormous importance, and

in particular the disposal of nuclear waste in solid form is of pressing concern.

The material in all of the later sections is founded upon the concepts presented in Part 1, that is, properties are explained as arising naturally from the atomic constituents, the chemical bonding, the microstructures and defects present in the solid. This leads naturally to an understanding of why nanostructures have seemingly different properties from bulk solids. Because of this, nanostructures are not gathered together in one section, but considered throughout the book, in the context of the better-known macroscopic properties of the material.

It is a pleasure to acknowledge the help of Dr A. Slade and Mrs Celia Carden of John Wiley, who

have given continual encouragement and assistance to this venture. Ms Rachael Catt read the complete manuscript with meticulous care, exposed ambiguities and inconsistencies in both text and figures, and added materially to the final version. Mr Allan Coughlin read large parts of earlier drafts, clarified many obscurities and suggested many improvements. Mr Rolfe Jones has provided information and micrographs of solids whenever called upon. As always, my family has been ever-supportive during the writing of this book, and my wife Anne has endured the hours of being a computer widow without complaint. To all of these, my heartfelt thanks.

PART 1

Structures and microstructures

1

The electron structure of atoms

- What is a wavefunction?
- What is an atomic term?
- How are the energy levels of atoms labelled?

The electrons associated with the chemical elements in a material (whether in the form of a gas, liquid or solid) control the chemical and physical properties of the atoms. The energies and regions of space occupied by electrons in an atom may be calculated using *quantum theory*.

1.1 The hydrogen atom

1.1.1 The quantum mechanical description

An atom of any element is made up of a small massive *nucleus*, in which almost all of the mass resides, surrounded by an *electron cloud*. Each element is differentiated from all others by the amount of positive charge on the nucleus, called the *proton number* or *atomic number*, Z . The proton number is an integer specifying the number of protons in the nucleus, each of which carries one unit of positive charge. In a neutral atom, the nuclear charge is exactly balanced by Z electrons in the outer electron cloud, each of which carries one unit of negative charge. Variants of atoms that have slightly more or fewer electrons than are required for charge neutrality are called *ions*; those which have lost electrons have an overall positive charge and those that have gained electrons have an overall negative charge. Positively charged ions are sometimes called *cations* and negatively charged ions are sometimes called *anions*.

A hydrogen atom is the simplest of atoms. It consists of a nucleus consisting of a single proton carrying one unit of positive charge, together with a single bound electron carrying one unit of negative charge. *Hydrogenic* or *hydrogen-like* atoms or ions are very similar, in that they can be analysed in terms of a single electron bound to a nucleus with an apparent charge different from unity. Information about the electron can be obtained by solving the *Schrödinger equation*, in which the electron is represented as a wave. The permitted solutions to this equation, called *wavefunctions*, describe the energy and probability of location of the electron in any region around the nucleus. Each of the solutions contains three integer terms called *quantum numbers*. They are n , the *principal quantum number*, l , the *orbital angular momentum quantum number*, and m_l , the *magnetic quantum number*. The names of the last two quantum numbers pre-date modern

quantum chemistry. They are best regarded as labels rather than representing classical concepts such as the angular momentum of a solid body. The quantum numbers define the *state* of a system.

1.1.2 The energy of the electron

The principal quantum number, n , defines the energy of the electron. It can take integer values 1, 2, 3 . . . to infinity. The energy of the electron is lowest for $n=1$ and this represents the most stable or *ground state* of the hydrogen atom. The next lowest energy is given by $n=2$, then by $n=3$, and so on. The energy of each state is given by the simple formula:

$$E = \frac{-A}{n^2} \quad (1.1)$$

where A is a constant equal to 2.179×10^{-18} J (13.6 eV),¹ and E is the energy of the level with principal quantum number n . The negative sign in the equation indicates that the energy of the electron is chosen as zero when n is infinite, that is to say, when the electron is no longer bound to the nucleus.

There is only one wavefunction for the lowest energy, $n=1$, state. The states of higher energy each have n^2 different wavefunctions, all of which have the same energy, that is, there are four different wavefunctions corresponding to $n=2$, nine different wavefunctions for $n=3$, and so on. These wavefunctions are differentiated from each other by different values of the quantum numbers l and m_l , as explained below. Wavefunctions with the same energy are said to be *degenerate*.

It is often convenient to represent the energy associated with each value of the principal quantum number, n , as a series of steps or *energy levels* (Figure 1.1). It is important to be aware of the fact that the electron can only take the exact energy values given by equation (1.1). When an electron gains energy, it jumps from an energy level with a lower value of n to a level with a higher value of n . When

¹ The unit of energy, *electron volt*, eV, is frequently used for atomic processes. $1\text{ eV} = 1.602 \times 10^{-19}\text{ J}$.

an electron loses energy, it drops from an energy level with a higher value of n to an energy level with a lower value. The discrete packets of energy given out or taken up in this way are *photons* of electromagnetic radiation (Chapter 14). The energy of a photon needed to excite an electron from energy E_1 , corresponding to an energy level n_1 , to energy E_2 , corresponding to an energy level n_2 , is given by:

$$\begin{aligned} E = E_1 - E_2 &= -2.179 \times 10^{-18} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \text{ J} \\ &= -13.6 \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \text{ eV} \end{aligned} \quad (1.2)$$

The energy of the photon emitted when the electron falls back from E_2 to E_1 is the same. The frequency, ν (or the equivalent wavelength, λ), of the photons that are either emitted or absorbed during these energy changes is given by the equation:

$$E = h\nu = \frac{hc}{\lambda} \quad (1.3)$$

where h is the Planck constant. (Note that this equation applies to the transition between any two

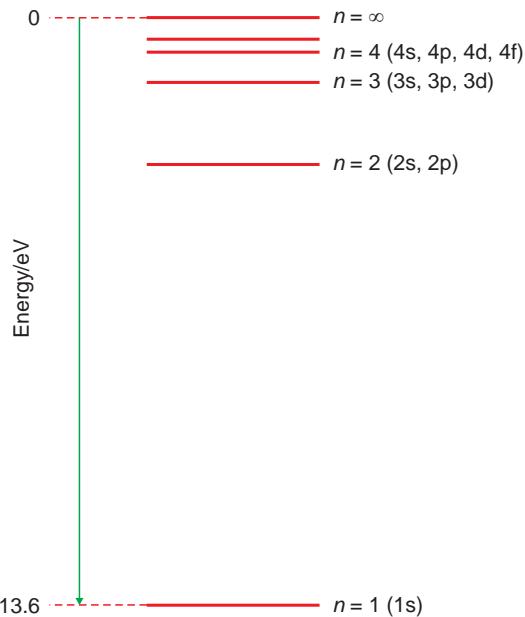


Figure 1.1 The energy levels available to an electron in a hydrogen atom.

energy levels on any atom, not just between energy levels on hydrogen or a hydrogenic atom.) The energy needed to free the electron completely from the proton, which is called the *ionisation energy* of the hydrogen atom, is given by putting $n_1 = 1$ and $n_2 = \infty$ in equation (1.2). The ionisation energy is 13.6 eV (2.179×10^{-18} J).

In the case of a single electron attracted to a nucleus of charge $+Ze$, the energy levels are given by:

$$E = \frac{-AZ^2}{n^2} \quad (1.4)$$

This shows that the energy levels are much lower than in hydrogen, and that the ionisation energy of such atoms is considerably higher.

1.1.3 Electron orbitals

The principal quantum number is not sufficient to determine the location of the electron in a hydrogen atom. In addition, the two other interdependent quantum numbers, l and m_l , are needed.

- l takes values of 0, 1, 2 . . . ($n - 1$)
- m_l takes values of 0, $\pm 1, \pm 2 \dots \pm l$

Each set of quantum numbers defines the *state* of the system and is associated with a wavefunction. For a value of $n = 1$, there is only one wavefunction, corresponding to $n = 1$, $l = 0$ and $m_l = 0$. For $n = 2$, l can take values of 0 and 1, and m_l can then take values of 0, associated with $l = 0$, and $-1, 0$ and $+1$, associated with $l = 1$. For $n = 3$, l can take values of 0, 1 and 2, and m_l then can take values of 0, associated with $l = 0, -1, 0$ and $+1$, associated with $l = 1$, and $-2, -1, 0, +1, +2$, associated with $l = 2$. These states are referred to as *orbitals* and for historical reasons they are given letter symbols. Orbitals with $l = 0$ are called *s orbitals*, those with $l = 1$ are called *p orbitals*, those with $l = 2$ are called *d orbitals*, and those with $l = 3$ are called *f orbitals* (Table 1.1).

The set of orbitals derived from a single value of the principal quantum number form a *shell*. The lowest energy shell is called the K shell, and corresponds to $n = 1$. The other shells are labelled alphabetically

Table 1.1 Quantum numbers and orbitals for the hydrogen atom

n	l	m_l	Orbital	Shell
1	0	0	1s	K
2	0	0	2s	L
		1	$-1, 0, +1$	2p (3 orbitals)
3	0	0	3s	M
		1	$-1, 0, +1$	3p (3 orbitals)
	2	$-2, -1, 0, +1, +2$	3d (5 orbitals)	
4	0	0	4s	N
	1	$-1, 0, +1$	4p (3 orbitals)	
	2	$-2, -1, 0, +1, +2$	4d (5 orbitals)	
	3	$-3, -2, -1, 0, +1, +2, +3$	4f (7 orbitals)	

(Table 1.1). For example, the L shell corresponds to the four orbitals associated with $n = 2$.

There is only one s orbital in any shell, labelled 1s, 2s and so on. There are three p orbitals in all shells from $n = 2$ upwards, collectively called 3p, 4p and so on. There are five d orbitals in the shells from $n = 3$ upwards, collectively called 3d, 4d, 5d and so on. There are seven f orbitals in the shells from $n = 4$ upwards, collectively called 4f, 5f and so on.

1.1.4 Orbital shapes

The *probability* of encountering the electron in a certain small volume of space surrounding a point with coordinates x , y and z is proportional to the square of the wavefunction at that point. With this information, it is possible to map out regions around the nucleus where the electron density is greatest.

The probability of encountering an electron in an s orbital does not depend upon direction but does vary with distance from the nucleus (Figure 1.2a,b,c). This probability peaks at a radial distance of 0.05292 nm for a 1s orbital – equal to the distance calculated by Bohr as the minimum allowed radius of an orbiting ‘planetary’ electron around a proton, and called the *Bohr radius*. As the electron is promoted to the 2s, 3s, 4s orbitals, the maximum probability peaks further and further from the nucleus. Thus a high-energy electron is most likely to be found far from the

nucleus. Generally, s orbitals are drawn as spherical *boundary surfaces* that enclose an arbitrary volume in which there is a high probability, say 95%, that the electron will be found (Figure 1.2d,e).

All other wavefunctions are specified by three quantum numbers and can be divided into two parts: a radial part, with similar probability shapes to those shown in Figure 1.2, multiplied by an angular part. The maximum probability of finding the electron depends upon both the radial and angular parts of the wavefunction, and the resulting boundary surfaces have complex shapes. For many purposes, however, it is sufficient to describe only the angular part of the wavefunction.

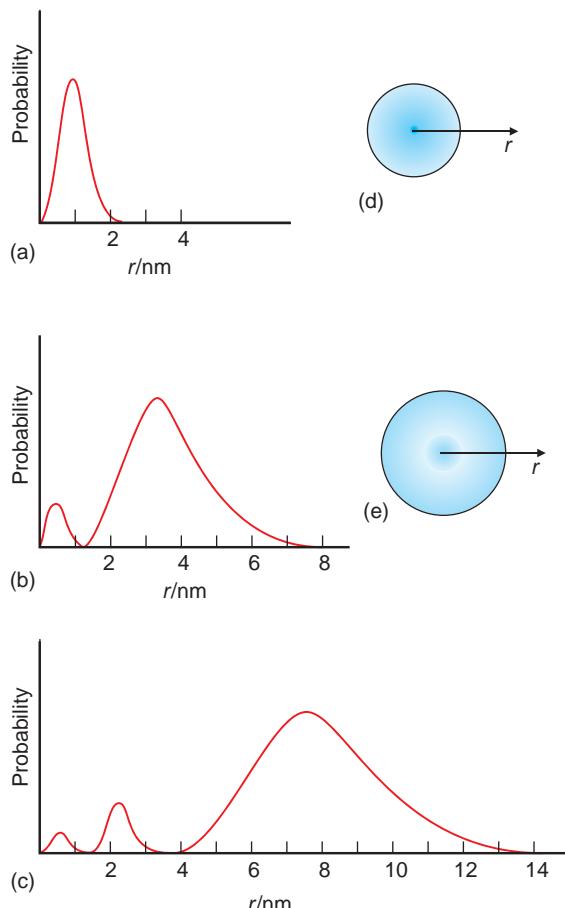


Figure 1.2 The probability of finding an electron at a distance r from the nucleus: (a) 1s; (b) 2s; (c) 3s. The boundary surfaces of the orbitals: (d) 1s; (e) 2s.

The boundary surfaces of the angular parts of the three p orbitals are approximately dumbbell-shaped, each consisting of two lobes. These lie along three mutually perpendicular directions, which it is natural to equate to x , y and z -axes (Figure 1.3). The corresponding orbitals are labelled np_x , np_y and np_z , for

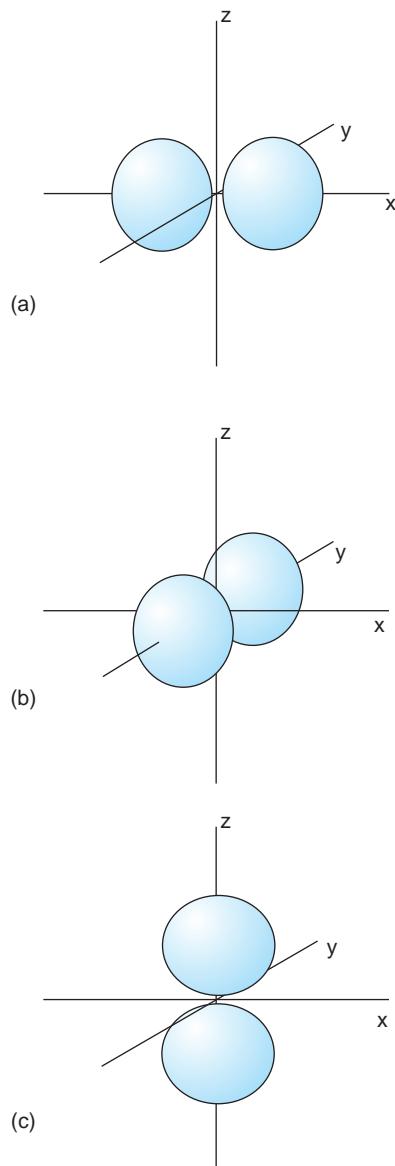


Figure 1.3 The boundary surfaces of the p orbitals: (a) p_x ; (b) p_y ; (c) p_z .

example, $2p_x$, $2p_y$ and $2p_z$. Note that the electron occupies both lobes of the p orbital. The probability of encountering a p electron on the perpendicular plane that separates the two halves of the dumbbell is zero, and this plane is called a *nodal plane*. The sign of the wavefunction is of importance when orbitals overlap to form bonds. The two lobes of each p orbital are labelled as + and −, and the sign changes as a nodal plane is crossed. The radial probability of encountering an electron in a p orbital is zero at the nucleus, and increases with distance from the nucleus. The maximum probability is further from the nucleus for an electron in a $3p$ orbital than a $2p$ orbital, and so on, so that $3p$ orbitals have a greater extension in space than $2p$ orbitals.

The distribution of the electron in either the d or f orbitals is more complicated than those of the p orbitals. There are five d orbitals, and seven f orbitals. Three of the $3d$ set of wavefunctions have lobes lying between pairs of axes, d_{xy} between the x - and y -axes, d_{xz} between the x - and z -axes, and d_{yz} between the y - and z -axes. The other two orbitals have lobes along the axes, $d_{x^2-y^2}$ pointing along x and y , and d_{z^2} pointing along the z -axis (Figure 1.4). Except for the d_{z^2} orbital, two perpendicular planar nodes separate the lobes and intersect at the nucleus. In the d_{z^2} orbital, the nodes are conical surfaces.

1.2 Many-electron atoms

1.2.1 The orbital approximation

If we want to know the energy levels and electron distribution of an atom with a nuclear charge of $+Z$ surrounded by Z electrons, it is necessary to write out a more extended form of the Schrödinger equation that takes into account not only the attraction of the nucleus for each electron, but also the repulsive interactions between the electrons themselves. The resulting equation has proved impossible to solve analytically, but increasingly accurate numerical solutions have been available for many years.

The simplest level of approximation, called the *orbital approximation*, supposes that an electron moves in a potential due to the nucleus and the average field of all the other electrons present in the

atom. This means that the electron experiences an *effective nuclear charge*, Z_{eff} , which is considered to be located as a point charge at the nucleus of the atom. In this approximation the orbital shapes are the same as for hydrogen, but the energy levels of all of the orbitals drop sharply as Z_{eff} increases (Figure 1.5). When one reaches lithium, $Z=3$, the $1s$ orbital energy has already decreased so much that it forms a chemically unreactive shell. This is translated into the concept of an atom as consisting of unreactive *core electrons*, surrounded by a small number of outermost *valence electrons*, which are of chemical significance. Moreover, the change of energy as Z increases justifies the approximation that the valence electrons of all atoms are at similar energies.

Although *shapes* of the orbitals are not changed from the shapes found for hydrogen, the radial part of the wave function is altered, and the *extension* of the orbitals increases as the effective nuclear charge increases. This corresponds to the idea that heavy atoms are larger than light atoms. In addition, a different effective nuclear charge is experienced by electrons in differing orbitals. This has the effect of separating the energy of the ns , np , nd and nf orbitals that are identical in hydrogen. It is found that for any value of n , the s orbitals have lowest energy, the three p orbitals have equal and slightly higher energy, the five d orbitals have equal and slightly higher energy again, and the seven f orbitals have equal and slightly higher energy again (Figure 1.6). However, the energy differences between the higher energy orbitals are very small, and this simple ordering is not followed exactly for heavier atoms.

1.2.2 Electron spin and electron configuration

The results presented so far, derived from solutions to the simplest form of the Schrödinger equation, do not explain the observed properties of atoms exactly. In order to account for the discrepancy the electron is allocated a fourth quantum number called the *spin quantum number*, s . The spin quantum number has a value of $\frac{1}{2}$. The spin of an electron on an atom

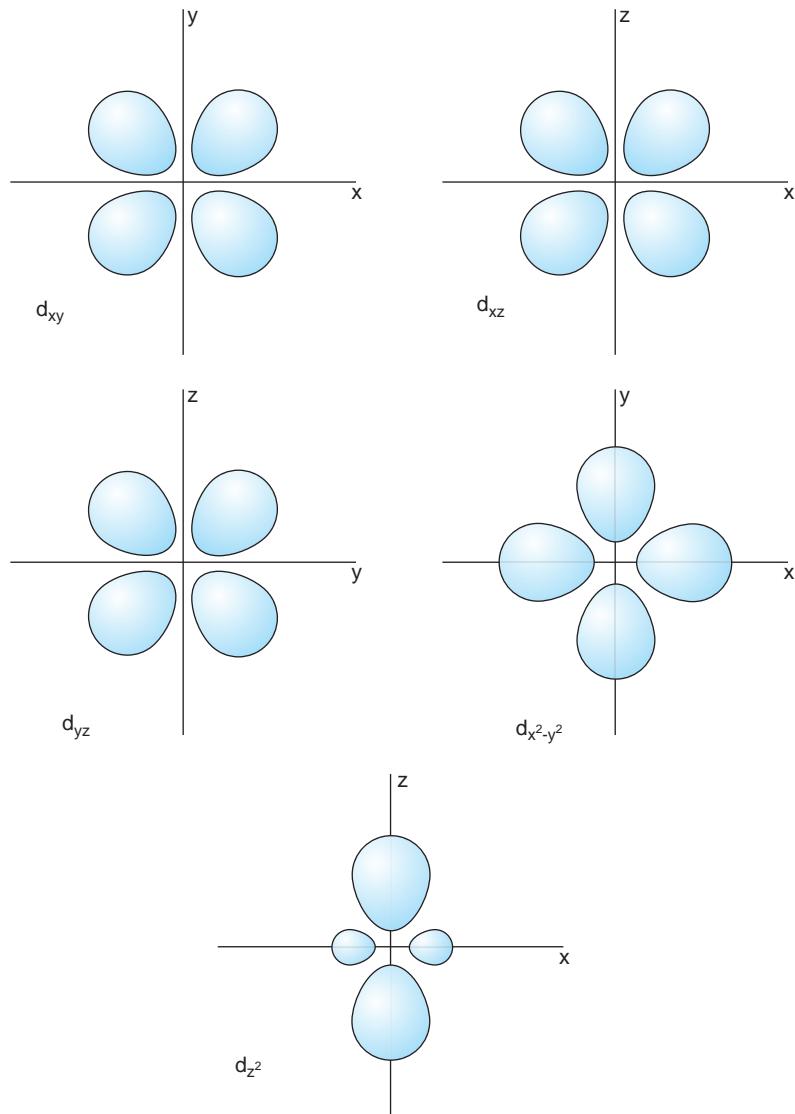


Figure 1.4 The boundary surfaces of the d orbitals: (a) d_{xy} ; (b) d_{xz} ; (c) d_{yz} ; (d) $d_{x^2-y^2}$; (e) d_{z^2} .

can adopt one of two different directions, represented by a quantum number, m_s , which takes values of $+1/2$ or $-1/2$. These two spin directions have considerable significance in chemistry and physics and are frequently represented by \uparrow , *spin up*, or α , and \downarrow , *spin down* or β . Although the spin quantum number was originally postulated to account for certain experimental observations, it arises naturally in

more sophisticated formulations of the Schrödinger equation that take into account the effects of relativity.

The *electron configuration* of an atom is the description of the number of electrons in each orbital, based upon the orbital model. This is usually given for the lowest energy possible, called the *ground state*. To obtain the electron configuration