

Structure of Materials

An Introduction to Crystallography, Diffraction and Symmetry

This highly readable, popular textbook for upper undergraduates and graduates comprehensively covers the fundamentals of crystallography, symmetry, and diffraction, and applies these concepts to a large range of materials. This edition now includes more streamlined coverage of crystallography, additional coverage of magnetic point group symmetry, and updated material on extraterrestrial minerals and rocks. New exercises at the end of chapters, plus over 500 exercises available online, allow students to check their understanding of key concepts and put into practice what they have learnt. Over 400 illustrations within the text help students visualize crystal structures and more abstract mathematical objects, supporting more difficult topics, such as point group symmetries. Historical and biographical sections add colour and interest by giving an insight into those who have contributed significantly to the field. Supplementary online material includes password-protected solutions, over 100 crystal structure data files, and PowerPoint files of figures from the book (available at www.cambridge.org/degraeef).

MARC DE GRAEF is a Professor in the Department of Materials Science and Engineering at the Carnegie Mellon University in Pittsburgh, USA, where he is also Co-director of the J. Earle and Mary Roberts Materials Characterization Laboratory. He received his Ph.D. in Physics in 1989 from the Catholic University of Leuven. An accomplished writer in the field, he is a Fellow of the Microscopy Society of America.

MICHAEL E. MCHENRY is Professor of Materials Science and Engineering, with an appointment in Physics, at the Carnegie Mellon University in Pittsburgh, USA. He received his Ph.D. in Materials Science and Engineering in 1988 from MIT, before which he spent three years working in industry as a Process Engineer. Also an accomplished writer, he is Publication Chair for the Magnetism and Magnetic Materials (MMM) Conference.

“This book is a lucid, modern, visually attractive exposition of the fascinating and perennially useful subject of the structure of materials. With examples from various materials classes, it will be a valuable addition to the library of most materials scientists and engineers.”

R.V. RAMANUJAN, Nanyang Technological University

“The book represents more than an introduction to crystallography, diffraction and symmetry. It is a thorough work explaining the structure of materials from the basic principles of crystallography and the techniques of characterization including analysis of representative materials (metals, ceramics, amorphous, molecular solids and nanomaterials). The easy reading together with the number of illustrations facilitates the understanding of complex structures. The book is a good reference, and the inclusion of problems at the end of each chapter makes it a very useful text book for beginners.”

MARINA DÍAZ MICHELENA, Instituto Nacional de Técnica Aeroespacial

“De Graef and McHenry have written a masterpiece in a rich and historical subject that is critical in understanding many topics in materials science and engineering, chemistry, physics, and geology. They provide a comprehensive and unified blend of underlying theory and practice using innumerable illustrations, micrographs, exercises, and other resources such as 3-D interactive software to aid in the visualization of crystal and molecular structures. This book can serve as an advanced undergraduate or a graduate text, as well as a comprehensive resource that everyone working in all aspects of material structure, diffraction science, and crystallography will want to own.”

THOMAS W. SCHARF, University of North Texas

Cambridge University Press
978-1-107-00587-7 — Structure of Materials
2nd Edition
Marc De Graef, Michael E. McHenry
Frontmatter
[More Information](#)

Structure of Materials

AN INTRODUCTION TO
CRYSTALLOGRAPHY, DIFFRACTION
AND SYMMETRY

MARC DE GRAEF

Carnegie Mellon University, Pittsburgh

MICHAEL E. McHENRY

Carnegie Mellon University, Pittsburgh

Second edition, fully revised and updated



CAMBRIDGE
UNIVERSITY PRESS

Cambridge University Press
 978-1-107-00587-7 — Structure of Materials
 2nd Edition
 Marc De Graef, Michael E. McHenry
 Frontmatter
[More Information](#)

CAMBRIDGE UNIVERSITY PRESS

University Printing House, Cambridge CB2 8BS, United Kingdom
 One Liberty Plaza, 20th Floor, New York, NY 10006, USA
 477 Williamstown Road, Port Melbourne, VIC 3207, Australia
 314-321, 3rd Floor, Plot 3, Splendor Forum, Jasola District Centre, New Delhi - 110025, India
 103 Penang Road, #05-06/07, Visioncrest Commercial, Singapore 238467

Cambridge University Press is part of the University of Cambridge.

It furthers the University's mission by disseminating knowledge in the pursuit of education, learning and research at the highest international levels of excellence.

www.cambridge.org

Information on this title: www.cambridge.org/9781107005877

© M. De Graef and M. McHenry 2007, 2012

This publication is in copyright. Subject to statutory exception and to the provisions of relevant collective licensing agreements, no reproduction of any part may take place without the written permission of Cambridge University Press.

First published 2007

Second edition first published 2012

8th printing 2020

A catalogue record for this publication is available from the British Library

Library of Congress Cataloging in Publication data

De Graef, Marc, author.

Structure of materials : an introduction to crystallography, diffraction and symmetry /

Marc De Graef, Carnegie Mellon University, Pittsburgh, Michael E. McHenry,

Carnegie Mellon University, Pittsburgh. –

[Second edition].

pages cm

ISBN 978-1-107-00587-7 (Hardback)

1. Crystallography. 2. Diffraction. 3. Symmetry. 4. Materials science.

I. McHenry, Michael E., author. II. Title.

QD911.D396 2012

548'.8–dc23

2012015928

ISBN 978-1-107-00587-7 Hardback

Additional resources for this publication at www.cambridge.org/9781107005877

Cambridge University Press has no responsibility for the persistence or accuracy of URLs for external or third-party internet websites referred to in this publication, and does not guarantee that any content on such websites is, or will remain, accurate or appropriate.

Cambridge University Press
978-1-107-00587-7 — Structure of Materials
2nd Edition
Marc De Graef , Michael E. McHenry
Frontmatter
[More Information](#)

In memory of Mary Ann (McHenry) Bialosky (1962–1999), a devoted teacher,
student, wife and mother, who was taken from us much too soon.

M.E.M.

For Marie, Pieter, and Erika.

M.D.G.

Contents

	Preface to the second edition	<i>page</i> xix
	Preface to the first edition	xxi
	Acknowledgements	xxv
	Figure reproductions	xxvii
	Symbols	xxix
1	Materials and material properties	1
1.1	Materials and structure	1
1.2	Organization of the book	2
1.3	About length scales	3
1.4	Wave–particle duality and the de Broglie relationship	7
1.5	What is a material property?	9
1.5.1	Definition of a material property	9
1.5.2	Directional dependence of properties	10
1.5.3	A first encounter with symmetry	12
1.5.4	A first encounter with magnetic symmetry	15
1.6	So, what is this book all about?	17
1.7	Chapter summary	19
1.8	Historical notes	20
1.9	Selected problems	21
2	The periodic table of the elements and interatomic bonds	23
2.1	About atoms	23
2.1.1	The electronic structure of the atom	23
2.1.2	The hydrogenic model	24
2.2	The periodic table	26
2.2.1	Layout of the periodic table	28
2.2.2	Trends across the table	31
2.3	Interatomic bonds	34
2.3.1	Quantum chemistry	34
2.3.2	Interactions between atoms	34
2.3.3	The ionic bond	36
2.3.4	The covalent bond	38
2.3.5	The metallic bond	39
2.3.6	The van der Waals bond	40
2.3.7	Mixed bonding	41
2.3.8	Electronic states and symmetry	41
2.3.9	Overview of bond types and material properties	42

Contents

2.4	Chapter summary	43
2.5	Historical notes	43
2.6	Selected problems	47
3	What is a crystal structure?	49
3.1	Periodic arrangements of atoms	49
3.2	The space lattice	51
3.2.1	Basis vectors and translation vectors	51
3.2.2	Some remarks about notation	52
3.2.3	More about lattices	54
3.3	The four 2-D crystal systems	56
3.4	The seven 3-D crystal systems	57
3.5	The five 2-D Bravais nets and fourteen 3-D Bravais lattices	60
3.6	Other ways to define a unit cell	64
3.7	*2-D and 3-D magnetic Bravais lattices	66
3.8	Chapter summary	71
3.9	Historical notes	72
3.10	Selected problems	73
4	Crystallographic computations	75
4.1	Directions in the crystal lattice	75
4.2	Distances and angles in a 3-D lattice	76
4.2.1	Distance between two points	76
4.2.2	The metric tensor	78
4.2.3	The dot product in a crystallographic reference frame	80
4.3	Worked examples	82
4.3.1	Computation of the length of a vector	82
4.3.2	Computation of the distance between two atoms	83
4.3.3	Computation of the angle between atomic bonds	84
4.3.4	Computation of the angle between lattice directions	84
4.3.5	An alternative method for the computation of angles	85
4.3.6	Further comments	85
4.4	Chapter summary	86
4.5	Historical notes	87
4.6	Selected problems	89
5	Lattice planes	90
5.1	Miller indices	90
5.2	Families of planes and directions	93
5.3	Special case: the hexagonal system	94
5.4	Crystal forms	96
5.5	Chapter summary	101
5.6	Historical notes	101
5.7	Selected problems	102

6	Reciprocal space	104
6.1	The reciprocal basis vectors	104
6.2	Reciprocal space and lattice planes	108
6.3	The reciprocal metric tensor	110
6.3.1	Computation of the angle between planes	112
6.3.2	Computation of the length of the reciprocal lattice vector	112
6.4	Worked examples	114
6.5	Chapter summary	119
6.6	Historical notes	119
6.7	Selected problems	120
7	Additional crystallographic computations	122
7.1	The stereographic projection	122
7.2	About zones and zone axes	125
7.2.1	The vector cross product	126
7.2.2	About zones and the zone equation	130
7.2.3	The reciprocal lattice and zone equation in the hexagonal system	131
7.3	Relations between direct space and reciprocal space	133
7.4	Coordinate transformations	135
7.4.1	Transformation rules	135
7.4.2	Example of a coordinate transformation	138
7.4.3	Converting vector components into Cartesian coordinates	140
7.5	Examples of stereographic projections	143
7.5.1	Stereographic projection of a cubic crystal	143
7.5.2	Stereographic projection of a monoclinic crystal	146
7.6	Chapter summary	149
7.7	Historical notes	150
7.8	Selected problems	151
8	Symmetry in crystallography	152
8.1	Symmetry of an arbitrary object	152
8.2	Symmetry operations	158
8.2.1	Basic isometric transformations	159
8.2.2	Compatibility of rotational symmetries with crystalline translational periodicity	160
8.2.3	Operations of the first kind: pure rotations	162
8.2.4	Operations of the first kind: pure translations	164
8.2.5	Operations of the second kind: pure reflections	166
8.2.6	Operations of the second kind: inversions	167
8.2.7	Symmetry operations that do not pass through the origin	168
8.3	*Magnetic symmetry operations	169
8.3.1	Time-reversal symmetry and axial vectors	169
8.3.2	Time-reversing symmetry operations	173
8.4	Combinations of symmetry operations	175
8.4.1	Combination of rotations with the inversion center	175

Contents

8.4.2	Combination of rotations and mirrors	177
8.4.3	Combination of rotations and translations	178
8.4.4	Combination of mirrors and translations	181
8.4.5	Relationships and differences between operations of the first and second kind	183
8.4.6	*Combinations of magnetic and regular symmetry operators	184
8.5	Point symmetry	186
8.6	Chapter summary	188
8.7	Historical notes	190
8.8	Selected problems	191
9	Point groups	193
9.1	What is a group?	193
9.1.1	A simple example	193
9.1.2	Group axioms	194
9.1.3	Principal properties of groups	196
9.2	3-D crystallographic point symmetries	197
9.2.1	Step I: the proper rotations	198
9.2.2	Step II: combining proper rotations with two-fold rotations	199
9.2.3	Step IIIa: combining proper rotations with inversion symmetry	201
9.2.4	Step IIIb: combining proper rotations with perpendicular reflection elements	203
9.2.5	Step IV: combining proper rotations with coinciding reflection elements	204
9.2.6	Step Va: combining inversion rotations with coinciding reflection elements	204
9.2.7	Step Vb: combining proper rotations with coinciding and perpendicular reflection elements	205
9.2.8	Step VI: combining proper rotations	206
9.2.9	Step VII: adding reflection elements to Step VI	207
9.2.10	General remarks	208
9.3	2-D crystallographic point symmetries	220
9.4	*Magnetic point groups	221
9.4.1	Derivation	221
9.4.2	Visualization of the magnetic point groups	223
9.4.3	Color, charge, and time reversal	225
9.5	Chapter summary	227
9.6	Historical notes	228
9.7	Selected problems	228
10	Plane groups and space groups	230
10.1	Combining translations with point group symmetry	230
10.2	Plane groups	231
10.2.1	A simple example	231
10.2.2	A more complex example	233

Contents

10.2.3	The 17 plane groups	235
10.3	Space groups	236
10.3.1	A simple example	236
10.3.2	A second simple example	238
10.3.3	A more complex example	239
10.3.4	The symmorphic space groups	240
10.3.5	The non-symmorphic space groups	242
10.3.6	*Space group generators	243
10.3.7	General remarks	247
10.4	The <i>International Tables for Crystallography</i>	248
10.5	*Magnetic space groups	253
10.6	Chapter summary	255
10.7	Historical notes	256
10.8	Selected problems	257
11	X-ray diffraction: geometry	259
11.1	Properties and generation of X-rays	259
11.1.1	How do we generate X-rays?	261
11.1.2	Wavelength selection	265
11.2	X-rays and crystal lattices	268
11.2.1	Scattering of X-rays by lattice planes	272
11.2.2	Bragg’s law in reciprocal space	276
11.3	Basic experimental X-ray diffraction techniques	280
11.3.1	The X-ray powder diffractometer	281
11.4	Chapter summary	289
11.5	Historical notes	289
11.6	Selected problems	290
12	X-ray diffraction: intensities	291
12.1	Scattering by electrons, atoms, and unit cells	291
12.1.1	Scattering by a single electron	291
12.1.2	Scattering by a single atom	293
12.1.3	Scattering by a single unit cell	298
12.2	The structure factor	300
12.2.1	Lattice centering and the structure factor	300
12.2.2	Symmetry and the structure factor	304
12.2.3	Systematic absences and the <i>International Tables for Crystallography</i>	307
12.2.4	Examples of structure factor calculations	307
12.3	Intensity calculations for diffracted and measured intensities	309
12.3.1	Description of the correction factors	310
12.3.2	Expressions for the total measured intensity	315
12.4	Chapter summary	317
12.5	Historical notes	317
12.6	Selected problems	318

13	Other diffraction techniques	320
13.1	Introductory remarks	320
13.2	*Neutron diffraction	321
13.2.1	Neutrons: generation and properties	323
13.2.2	Neutrons: wavelength selection	325
13.2.3	Neutrons: atomic scattering factors	326
13.2.4	Neutrons: scattering geometry and diffracted intensities	330
13.2.5	Neutrons: example powder pattern	334
13.3	*Electron diffraction	335
13.3.1	The electron as a particle and a wave	335
13.3.2	The geometry of electron diffraction	337
13.3.3	The transmission electron microscope	338
13.3.4	Basic observation modes in the TEM	340
13.3.5	Convergent beam electron diffraction	343
13.4	*Synchrotron X-ray sources for scattering experiments	347
13.4.1	Synchrotron accelerators	348
13.4.2	Synchrotron radiation: experimental examples	350
13.5	Chapter summary	352
13.6	Historical notes	352
13.7	Selected problems	354
14	About crystal structures and diffraction patterns	356
14.1	Crystal structure descriptions	356
14.1.1	Space group description	356
14.1.2	Graphical representation methods	357
14.2	Crystal structures ↔ powder diffraction patterns	360
14.2.1	The Ni powder pattern, starting from the known structure	361
14.2.2	The NaCl powder pattern, starting from the known structure	365
14.2.3	The Ni structure, starting from the experimental powder diffraction pattern	369
14.2.4	The NaCl structure, starting from the experimental powder diffraction pattern	372
14.2.5	*General comments about crystal structure determination	375
14.3	Chapter summary	380
14.4	Historical notes	380
14.5	Selected problems	382
15	Non-crystallographic point groups	383
15.1	Example of a non-crystallographic point group symmetry	383
15.2	Icosahedral and related five-fold symmetry groups	384
15.2.1	The icosahedral point groups	384
15.2.2	Fullerene molecular structures	385
15.2.3	Icosahedral group representations	387
15.2.4	Other non-crystallographic point groups with five-fold symmetries	390
15.2.5	Descents in symmetry: decagonal and pentagonal groups	393

15.3	Non-crystallographic point groups with octagonal symmetry	395
15.4	Chapter summary	400
15.5	Historical notes	400
15.6	Selected problems	402
16	Periodic and aperiodic tilings	403
16.1	2-D plane tilings	403
16.1.1	2-D regular tilings	404
16.1.2	2-D Archimedean tilings	405
16.1.3	k -uniform regular tilings	406
16.1.4	Dual tilings – the Laves tilings	407
16.1.5	Tilings without regular vertices	408
16.2	*Color tilings	408
16.3	*Quasiperiodic tilings	410
16.4	*Regular polyhedra and n -D regular polytopes	411
16.5	Crystals with stacking of 3^6 tilings	415
16.5.1	Simple close-packed structures: <i>ABC</i> stacking	415
16.5.2	Interstitial sites in close-packed structures	416
16.5.3	Representation of close-packed structures	417
16.5.4	Polytypism and properties of SiC semiconductors	419
16.5.5	3^6 close-packed tilings of polyhedral faces	420
16.6	Chapter summary	421
16.7	Historical notes	422
16.8	Selected problems	424
17	Metallic structures I: simple, derivative, and superlattice structures	425
17.1	Introductory comments	425
17.2	Classification of structures	426
17.2.1	Strukturbericht symbols	426
17.2.2	Pearson symbols	427
17.2.3	Structure descriptions in this book	427
17.3	Parent structures	428
17.3.1	Geometrical calculations for cubic structures	430
17.4	Atomic sizes, bonding, and alloy structure	431
17.4.1	Hume-Rothery rules	432
17.4.2	Bonding in close-packed rare gas and metallic structures	433
17.4.3	Phase diagrams	437
17.5	Superlattices and sublattices: mathematical definition	438
17.6	Derivative structures and superlattice examples	439
17.6.1	<i>fcc</i> -derived structures and superlattices	439
17.6.2	<i>bcc</i> -derived superlattices	444
17.6.3	Diamond cubic derived superlattices	446
17.6.4	Hexagonal close-packed derived superlattices	448
17.7	Elements with alternative stacking sequences or lower symmetry	450

17.7.1	Elements with alternative stacking sequences	450
17.7.2	Elements with lower-symmetry structures	451
17.8	*Natural and artificial superlattices	455
17.8.1	Superlattice structures based on the $L1_2$ cell	455
17.8.2	Artificial superlattices	457
17.8.3	X-ray scattering from long-period multi-layered systems	459
17.8.4	Incommensurate superlattices	459
17.9	Interstitial alloys	461
17.10	Chapter summary	462
17.11	Historical notes	463
17.12	Selected problems	464
18	Metallic structures II: complex geometrically determined structures	466
18.1	Electronic states in metals	466
18.2	Topological close packing	468
18.2.1	The Kasper polyhedra	469
18.2.2	Connectivity of Kasper polyhedra	471
18.2.3	Metallic radii	471
18.3	*Frank–Kasper alloy phases	472
18.3.1	A15 phases and related structures	472
18.3.2	The Laves phases and related structures	479
18.3.3	The sigma phase	486
18.3.4	The μ -phase and the M -, P -, and R -phases	488
18.4	*Quasicrystal approximants	490
18.4.1	$Mg_{32}(Al,Zn)_{49}$ and α -Al–Mn–Si crystal structures	490
18.4.2	$Mg_{32}(Al,Zn)_{49}$ and α -Al–Mn–Si shell models	491
18.5	Chapter summary	494
18.6	Historical notes	495
18.7	Selected problems	496
19	Metallic structures III: quasicrystals	497
19.1	Introductory remarks	497
19.2	The golden mean and pentagonal symmetry	498
19.3	1-D quasicrystals	501
19.3.1	The Fibonacci sequence and lattice derived by recursion	501
19.3.2	Lattice positions in the Fibonacci lattice	503
19.3.3	Construction of the Fibonacci lattice by the projection method	504
19.3.4	*The Fourier transform of the Fibonacci lattice	505
19.4	*2-D quasicrystals	507
19.4.1	2-D quasicrystals: Penrose tilings	507
19.4.2	The Penrose tiling derived by projection	512
19.4.3	2-D quasicrystals: other polygonal quasicrystals	514
19.5	*3-D quasicrystals	516
19.5.1	3-D Penrose tilings	517

Contents

19.5.2	Indexing icosahedral quasicrystal diffraction patterns	519
19.5.3	Icosahedral quasicrystal diffraction patterns and quasilattice constants	521
19.5.4	3-D Penrose tiles: stacking, decoration, and quasilattice constants	522
19.5.5	3-D Penrose tiles: projection method	524
19.6	*Multiple twinning and icosahedral glass models	525
19.7	*Microscopic observations of quasicrystal morphologies	526
19.8	Chapter summary	528
19.9	Historical notes	528
19.10	Selected problems	530
20	Metallic structures IV: amorphous metals	531
20.1	Introductory comments	531
20.2	Order in amorphous and nanocrystalline alloys	532
20.3	Atomic positions in amorphous alloys	535
20.4	Atomic volume, packing, and bonding in amorphous solids	536
20.4.1	DRPHS model	537
20.4.2	Binding in clusters: crystalline and icosahedral short-range order	539
20.4.3	Icosahedral short-range order models	539
20.5	Amorphous metal synthesis	540
20.6	Thermodynamic and kinetic criteria for glass formation	542
20.7	Examples of amorphous metal alloy systems	543
20.7.1	Metal–metalloid systems	544
20.7.2	Rare earth–transition metal systems	545
20.7.3	Early transition metal–late transition metal systems	546
20.7.4	Multi-component nanocomposite systems.	546
20.7.5	Multi-component bulk amorphous systems	548
20.8	*X-ray scattering in amorphous materials	550
20.9	*Extended X-ray absorption fine structure (EXAFS)	554
20.10	Mössbauer spectroscopy	557
20.11	Chapter summary	558
20.12	Historical notes	558
20.13	Selected problems	560
21	Ceramic structures I: basic structure prototypes	561
21.1	Introductory remarks	561
21.2	Ionic radii	562
21.3	Bonding energetics in ionic structures	565
21.4	Rules for packing and connectivity in ionic crystals	566
21.4.1	Pauling’s rules for ionic structures	566
21.4.2	Radius ratio rules for ionic compounds	567
21.5	Oxides of iron	570
21.6	Halide salt structures: CsCl, NaCl, and CaF ₂	571
21.7	Close-packed sulfide and oxide structures: ZnS and Al ₂ O ₃	574

21.8	Perovskite and spinel structures	577
21.8.1	Perovskites: ABO_3	577
21.8.2	Spinel: AB_2O_4	580
21.9	Non-cubic close-packed structures: NiAs, CdI_2 , and TiO_2	584
21.10	*Layered structures	585
21.10.1	Magnetoplumbite phases	586
21.10.2	Aurivillius phases	586
21.10.3	Ruddlesden–Popper phases	588
21.10.4	Tungsten bronzes	589
21.10.5	Titanium carbosulfide	591
21.11	Additional remarks	591
21.12	*Point defects in ceramics	592
21.13	Chapter summary	594
21.14	Historical notes	594
21.15	Selected problems	596
22	Ceramic structures II: high-temperature superconductors	597
22.1	Introductory remarks about superconductivity	597
22.2	High-temperature superconductors: nomenclature	598
22.3	*Perovskite-based high-temperature superconductors	599
22.3.1	Single-layer perovskite high-temperature superconductors	599
22.3.2	Triple-layer perovskite-based high-temperature superconductors	601
22.4	*BSCCO, TBCCO, HBCCO, and ACBCCO HTSC layered structures	606
22.4.1	The BSCCO double-layer high-temperature superconductors	606
22.4.2	The TBCCO double-layer high-temperature superconductors	608
22.4.3	The TBCCO single-layer high-temperature superconductors	611
22.4.4	The HBCCO high-temperature superconductors	613
22.4.5	The ACBCCO high-temperature superconductors	615
22.4.6	Rutheno-cuprate high-temperature superconductors	615
22.4.7	Infinite-layer high-temperature superconductors	616
22.5	Chapter summary	616
22.6	Historical notes	617
22.7	Selected problems	619
23	Ceramic structures III: terrestrial and extraterrestrial minerals	620
23.1	Classification of minerals	620
23.2	Silicates overview	622
23.2.1	Orthosilicates (nesosilicates)	624
23.2.2	Pyrosilicates (sorosilicates)	629
23.2.3	Chains of tetrahedra, metasilicates (inosilicates)	630
23.2.4	Double chains of tetrahedra	633
23.2.5	Sheets of tetrahedra, phyllosilicates	634
23.2.6	Networks of tetrahedra, tectosilicates	635
23.2.7	Random networks of tetrahedra: silicate glasses	639

23.2.8 Mesoporous silicates	641
23.2.9 Sol-gel synthesis of silicate nanostructures	642
23.3 Magnetic minerals on Mars and their biogenic origins	643
23.3.1 Hydroxides	646
23.3.2 Sulfates	649
23.4 Chapter summary	650
23.5 Historical notes	651
23.6 Selected problems	652
24 Molecular solids and biological materials	653
24.1 Introductory remarks	653
24.2 Simple molecular crystals: ice, dry ice, benzene, the clathrates, and self-assembled structures	654
24.2.1 Solid H ₂ O: ice	654
24.2.2 Solid CO ₂ : dry ice	656
24.2.3 Hydrocarbon crystals	657
24.2.4 Clathrates	658
24.2.5 Amphiphiles and micelles	659
24.3 Polymers	660
24.3.1 Polymer classification	661
24.3.2 Polymerization reactions and products	662
24.3.3 Polymer chains: spatial configurations	664
24.3.4 Copolymers and self-assembly	666
24.3.5 Conducting and superconducting polymers	668
24.3.6 Polymeric derivatives of fullerenes	670
24.4 Biological macromolecules	671
24.4.1 DNA and RNA	671
24.4.2 Virus structures	674
24.5 Fullerene-based molecular solids	677
24.5.1 Fullerites	679
24.5.2 Fullerides	681
24.5.3 Carbon nanotubes	681
24.6 Chapter summary	685
24.7 Historical notes	685
24.8 Selected problems	687
References	688
Index	716

Preface to the second edition

We are grateful to the many readers, students and teachers alike, who have sent us comments and corrections, or who simply expressed their appreciation of the first edition of our book. As always, it is difficult, if not impossible, to please everyone and to accommodate all requests for changes or additional material. As we prepared this second edition of *Structure of Materials*, we attempted simultaneously to shorten the text and make it more complete by adding sections on magnetic symmetry (time-reversal symmetry, magnetic Bravais lattices, and magnetic point and space groups). The new text has 24 chapters, as before split into 1–13 (crystallography and symmetry) and 15–24 (examples of important structures), with Chapter 14 as a transition chapter, applying the material from the first half of the book. In addition to the new material on magnetic symmetry, we have added sections on the oxides of iron (Chapter 21) and magnetic minerals on Mars (Chapter 23), and we have made numerous small changes throughout the text. The resulting text is more succinct, and, we hope, a significant improvement over the first edition.

Each chapter now has an introductory and summary section, and a short set of four new problems. Additional new problems, as well as all the problems from the first edition, can be found on the book's website, <http://som.web.cmu.edu/>, for a total of nearly 600 problems. Solution sets to all problems are made available to instructors via the publisher. In addition, PowerPoint files with enlarged versions (some in color) of all the figures from the book are available from the website. We hope that these files will become a valuable teaching resource.

The 2011 Nobel prize in chemistry was awarded to D. Shechtman for his discovery of quasicrystals, which prompted us to update the historical section of Chapter 19. This award is a testament to the importance of crystal structures in modern science and engineering; it should serve as a reminder that even after decades or centuries of steady scientific progress, unexpected discoveries occur every now and then that force a review, and in this case a *redefinition*, of the basic assumptions of a field. We hope that the interested reader will always keep an open mind when reading our text; while most of the material has stood the test of time (and scientific scrutiny), there is no telling which aspects of this book may need to be redefined at some point in the future. This constant questioning of the validity of basic scientific assumptions also means that this book is, in a way, just a 2011 snapshot of the field of crystallography; we sincerely hope that this snapshot will serve our readers and we will be pleased if, in any way, we can stimulate new discoveries that cause us to extend and reinterpret this field.

Preface to the first edition

In the movie *Shadowlands*,¹ Anthony Hopkins plays the role of the famous writer and educator, C. S. Lewis. In one scene, Lewis asks a probing question of a student: “*Why do we read?*” (Which could very well be rephrased: *Why do we study?* or *Why do we learn?*) The answer given is simple and provocative: “*We read to know that we are not alone.*” It is comforting to view education in this light. In our search to know that we are not alone, we connect our thoughts, ideas, and struggles to the thoughts, ideas, and struggles of those who preceded us. We leave our own thoughts for those who will follow us, so that they, too, will know that they are not alone. In developing the subject matter covered in this book, we (MEM and MDG) were both humbled and inspired by the achievements of the great philosophers, mathematicians, and scientists who have contributed to this field. It is our fervent hope that this text will, in some measure, inspire new students to connect their own thoughts and ideas with those of the great thinkers who have struggled before them and leave new ideas for those who will struggle afterwards.

The title of this book (*Structure of Materials*) reflects our attempt to examine the atomic structure of solids in a broader realm than just traditional crystallography, as has been suggested by Alan Mackay (1975). By combining visual illustrations of crystal structures with the mathematical constructs of crystallography, we find ourselves in a position to *understand* the complex structures of many modern engineering materials, as well as the structures of naturally occurring crystals and crystalline biological and organic materials. That all important materials are not crystalline is reflected in the discussion of amorphous metals, ceramics, and polymers. The inclusion of quasicrystals conveys the recent understanding that materials possessing long-range orientational order without 3-D translational periodicity must be included in a modern discussion of the structure of materials. The discovery of quasicrystals has caused the International Union of Crystallographers to redefine the term *crystal* as “any solid having an essentially discrete diffraction pattern.” This emphasizes the importance of diffraction theory and diffraction experiments in determining structure. It also means that extensions of the crystallographic theory to higher-dimensional spaces are necessary for the correct interpretation of the structure of quasicrystals.

Modern crystallography education has benefited tremendously from the availability of fast desktop computers; this book would not have been possible without the availability of wonderful free and commercial software for the visualization of crystal and molecular structures, for the computation of powder and single crystal diffraction patterns, and a host of other operations that would be nearly impossible to carry out by hand. We believe that the reader of this book will have an advantage over students of just a generation ago; he/she will be able to directly visualize all the crystal structures described in this text, simply by

¹ MEM is grateful to his good friend Joanne Bassilious for recommending this inspirational movie.

entering them into one of these visualization programs. The impact of visual aids should not be underestimated, and we have tried our best to include clear illustrations for more than 100 crystal structures. The structure files, available from the book's website, will be useful to the reader who wishes to look at these structures interactively.

About the structure of this book

The first half of the book, Chapters 1 through 13, deals with the basics of crystallography. It covers those aspects of crystallography that are mostly independent of any actual material, although we make frequent use of actual materials as examples, to clarify certain concepts and as illustrations. In these chapters, we define the seven crystal systems and illustrate how lattice geometry computations (bond distances and angles) can be performed using the metric tensor concept. We introduce the reciprocal space description and associated geometrical considerations. Symmetry operations are an essential ingredient for the description of a crystal structure, and we enumerate all the important symmetry elements. We show how sets of symmetry elements, called point groups and space groups, can be used to describe crystal structures succinctly. We introduce several concepts of diffraction, in particular the structure factor, and illustrate how the *International Tables for Crystallography* can be used effectively.

In the second half of the book, Chapters 15 through 25, we look at the structures of broad classes of materials. In these chapters, we consider, among others, metals, oxides, and molecular solids. The subject matter is presented so as to build an understanding of simple to more complex atomic structures, as well as to illustrate technologically important materials. In these later chapters, we introduce many geometrical principles that can be used to understand the structure of materials. These geometrical principles, which enrich the material presented in Chapters 1 through 13, also allow us to gain insight into the structure of quasicrystalline and amorphous materials, discussed in advanced chapters in the latter part of the text.

In the later chapters, we give examples of crystallographic computations that make use of the material presented in the earlier chapters. We illustrate the relationship between structures and phases of matter, allowing us to make elementary contact with the concept of a *phase diagram*. Phase relations and phase diagrams combine knowledge of structure with concepts from thermodynamics; typically, a thermodynamics course is a concurrent or subsequent part of the curriculum of a materials scientist or engineer, so that the inclusion of simple phase diagrams in this text strengthens the link with thermodynamics. Prominent among the tools of a materials scientist are those that allow the examination of structures on the nanoscale. Chapters in the latter half of the book have numerous illustrations of interesting nanostructures, presented as extensions to the topical discussions.

Chapter 14 forms the connection between the two halves of the book: it illustrates how to use the techniques of the first half to study the structures of the second half. We describe this connection by means of four different materials, which are introduced at the end of the first chapter. Chapter 14 also reproduces one of the very first scientific papers on the determination of crystal structures, the 1913 paper by W. H. Bragg and W. L. Bragg on *The Structure of the Diamond*. This seminal paper serves as an illustration of the long path that scientists have traveled in nearly a century of crystal structure determinations.

Some topics in this book are more advanced than others, and we have indicated these sections with an asterisk at the start of the section title. The subjects covered in each chapter are further amplified by 400 end-of-chapter reader exercises. At the end of each chapter, we have included a short historical note, highlighting how a given topic evolved, listing who did what in a particular subfield of crystallography, or giving biographical information on important crystallographers. Important contributors to the field form the main focus of these historical notes. The selection of contributors is not chronological and reflects mostly our own interests.

We have used the text of this book (in course-note form) for the past 13 years for a sophomore-level course on the structure of materials. This course has been the main inspiration for the book; many of the students have been eager to provide us with feedback on a variety of topics, ranging from “This figure doesn’t work,” to “Now I understand!” Developing the chapters of the book has also affected other aspects of the Materials Science and Engineering curriculum at CMU, including undergraduate laboratory experiments on amorphous metals, magnetic oxides, and high-temperature superconductors. Beginning in June, 1995, in conjunction with the CMU Courseware Development Program, multi-media modules for undergraduate students studying crystallography were created. The first module, “Minerals and Gemstones,” coupled photographic slides generously donated by Marc Wilson, curator of the Carnegie Museum of Natural History’s Hillman Hall of Minerals and Gems (in Pittsburgh, PA), with crystal shapes and atomic arrangements. This and subsequent software modules were made available on a CD in the fall of 1996; as updated versions become available, they will be downloadable through the book’s website. This software development work was heavily supported by our undergraduate students, and helped to shape the focus of the text. A module on the “History of Crystallography” served as a draft for the historical notes sections of this book.

The text can be used for a one-semester graduate or undergraduate course on crystallography; assuming a 14-week semester, with two 90-minute sessions per week, it should be possible to cover Chapters 1 through 14 in the first 11–12 weeks, followed by selected sections from the later chapters in the remainder of the semester. The second half of the book is not necessarily meant to be taught “as is”; instead, sections or illustrations can be pulled from the second half and used at various places in the first half of the book. Many of the reader exercises in the second half deal with the concepts of the first half.

Software used in the preparation of this book

Some readers might find it interesting to know which software packages were used for this book. The following list provides the name of the software package and the vendor (for commercial packages) or author website. Weblinks to all companies are provided through the book’s website.

- **Commercial packages:**
 - Adobe Illustrator [www.adobe.com];
 - Adobe Photoshop [www.adobe.com];
 - CrystalMaker and CrystalDiffract [www.crystallmaker.com].

Preface to the first edition

- **Shareware packages:**
 - QuasiTiler [www.geom.uiuc.edu/apps/quasitiler];
 - Kaleidotile (Version 1.5) [<http://geometrygames.org>].
- **Free packages:**
 - $\text{te}\text{T}\text{E}\text{X}$ [www.tug.org];
 - TeXShop [www.texshop.org];
 - POV-Ray [www.povray.org].

The website for this book runs on a dedicated Linux workstation located in MDG's office. The site can be reached through the publisher's website, or, directly, at <http://som.web.cmu.edu/>.

Acknowledgements

Many people have (knowingly or unknowingly) contributed to this book. We would like to thank as many of them as we can remember and apologize to anyone whom we have inadvertently forgotten. First of all, we would like to express our sincere gratitude to the many teachers who first instructed us in the field of the structure of materials. Michael McHenry's work on the subject of quasicrystals and icosahedral group theory dates back to his Massachusetts Institute of Technology (MIT) thesis research (McHenry, 1988). Michael McHenry acknowledges Professor Linn Hobbs, formerly of Case Western Reserve University and now at MIT, for his 1979 course *Diffraction Principles and Materials Applications* and the excellent course notes that have served to shape several of the topics presented in this text. Michael McHenry also acknowledges Professor Bernard Wuensch of MIT for his 1983 course *Structure of Materials*, which also served as the foundation for much of the discussion as well as the title of the book. The course notes from Professor Mildred Dresselhaus' 1984 MIT course *Applications of Group Theory to the Physics of Solids* also continue to inspire. Michael McHenry's course project for this course involved examining icosahedral group theory, and was suggested to him by his thesis supervisor, Robert C. O'Handley; this project has also had a profound impact on his future work and the choice of topics in this book.

Marc De Graef's first exposure to crystallography and diffraction took place in his second year of undergraduate studies in physics, at the University of Antwerp (Belgium), in a course on basic crystallography, taught by Professor J. Van Landuyt and Professor G. Van Tendeloo, and in an advanced diffraction course, also taught by Van Landuyt. Marc De Graef would also like to acknowledge the late Professor R. Gevers, whose course on analytical mechanics and tensor calculus proved to be quite useful for crystallographic computations as well. After completing a Ph.D. thesis at the Catholic University of Leuven (Belgium), MDG moved to the Materials Department at UCSB, where the first drafts of several chapters for this book were written. In 1993, he moved to the Materials Science and Engineering Department at Carnegie Mellon University, Pittsburgh, where the bulk of this book was written.

We are especially grateful to Professor Jose Lima-de-Faria for providing us with many of the photographs of crystallographers that appear in the historical notes sections of the book, as well as many others cited below. His unselfish love for the field gave the writers an incentive to try to emulate his wonderful work.

We would like to acknowledge the original students who contributed their time and skills to the multi-media courseware project: M.L. Storch, D. Schmidt, K. Gallagher, and J. Cheney. We offer our sincere thanks to those who have proofread chapters of the text. In particular, we thank Nicole Hayward for critically reading many chapters and for making significant suggestions to improve grammar, sentence structure, and so on. In addition, we would like to thank Matthew Willard, Raja Swaminathan, Shannon Willoughby, and Dan Schmidt for reading multiple chapters; and Sirisha Kuchimanchi, Julia Hess,

Acknowledgements

Paul Ohodnicki, Roberta Sutton, Frank Johnson, and Vince Harris for critical reading and commenting on selected chapters. We also thank our colleague Professor David Laughlin for critical input on several subjects and his contribution to a special tutorial at the 2000 Fall Meeting of The Minerals, Metals & Materials Society (TMS), “A Crystallography and Diffraction Tutorial Sponsored by the ASM-MSCTS Structures Committee.” We thank Marina Diaz-Michelena of INTA for introducing us to the magnetic minerals on Mars.

There is a large amount of literature on the subject of structure, diffraction, and crystallography. We have attempted to cite a manageable number of representative papers in the field. Because of personal familiarity with many of the works cited, our choices may have overlooked important works and included topics without full citations of *all* seminal books and papers in that particular area. We would like to apologize to those readers who have contributed to the knowledge in this field, but do not find their work cited. The omissions do not reflect on the quality of their work, but are a simple consequence of the human limitations of the authors.

The authors would like to acknowledge support from the National Science Foundation (NSF), grant nos. #1106943, #0804020 and #1005330, Los Alamos National Laboratory (LANL), the Air Force Office of Scientific Research (AFOSR), and Carnegie Mellon University for providing financial support during the writing of this book.

We would also like to thank several of our colleagues, currently or formerly at CMU, for their support during the years it has taken to complete the text: Greg Rohrer, Tresa Pollock, David Laughlin, and Alan Cramb. In particular, we would like to thank Jason Wolf, supervisor of the X-ray Diffraction facility; Tom Nuhfer, supervisor of the Electron Optics facility; and Bill Pingitore, MSE undergraduate laboratory technician at CMU.

We would like to thank our editors at Cambridge University Press, Tim Fishlock, Simon Capelin, Michelle Carey, and Anna Littlewood for their patience. This book has taken quite a bit longer to complete than we had originally anticipated, and there was no pressure to hurry up and finish it off. In this time of deadlines and fast responses, it was actually refreshing to be able to take the time needed to write and rewrite (and, often, rewrite again) the various sections of this book.

Marc De Graef would like to thank his wife, Marie, for her patience and understanding during the many years of evening and weekend work; without her continued support (and sporadic interest as a geologist) this book would not have been possible. Last but not least, the authors acknowledge their children. Michael McHenry’s daughter Meghan and son Michael lived through all of the travails of writing this book. Meghan’s friendship while a student at CMU has helped to further kindle the author’s interest in undergraduate education. Her friends represent the best of the intellectual curiosity that can be found in the undergraduates at CMU. Michael has developed an interest in computer networking and helped to solve many problems that only an adept young mind can grasp. We hope that he finds the joy in continued education that his sister has.

Both of Marc De Graef’s children, Pieter and Erika, were born during the writing of this book, so they have lived their entire lives surrounded by crystallographic paraphernalia; indeed, many of their childhood drawings, to this day, are made on the back of sheets containing chapter drafts and trial figures. Hopefully, at some point in the future, they will turn those pages and become interested in the front as well.

Figure reproductions

This book on the structure of materials has been enriched by the courtesy of other scientists in the field. A number of figures were taken from other authors' published or unpublished work, and the following acknowledgements must be made:

The following figures were obtained from J. Lima-de-Faria and are reproduced with his permission: 1.8(a),(b); 3.19(a), (b); 4.5(a),(b); 5.11(a),(b); 6.4(a),(b); 7.12(a),(b); 8.28(a),(b); 9.18(b); 10.14(a),(b); 15.16(a); 16.18(a),(b); 20.18(a),(b); 21.24(a); 23.28(a),(b).

The following figures were reproduced from the book *Introduction to Conventional Transmission Electron Microscopy* by M. De Graef (2003) with permission from Cambridge University Press: 3.3; 5.7; 7.1; 7.7; 7.8; 7.10; 8.20; 11.16; 13.5; 13.6; 13.8(a); 13.10; 13.11; 13.12.

Insets in Fig. 1.2 courtesy of D. Wilson, R. Rohrer, and R. Swaminathan; Fig. 11.8 courtesy of the Institute for Chemical Education; Fig. 13.13 courtesy of ANL; Fig. 13.14(a) photo courtesy of ANL, (b) picture courtesy of BNL; Fig. 13.16(b) courtesy of ANL; Fig. 13.17(a) courtesy of A. Hsiao and (b) courtesy of M. Willard; Figure in Box 16.1 courtesy of M. Skowronski; Figure in Box 17.1 courtesy of M. Tanase, D.E. Laughlin, and J.-G. Zhu; Fig. 17.29(a) courtesy of Department of Materials, University of Oxford; Fig. 17.29(b) courtesy of T. Massalski; Figure in Box 18.1 courtesy of E. Shevshenko and Chris Murray, IBM; Fig. 18.29(a) courtesy of the Materials Research Society, Warrendale, PA; Fig. 18.29(b) courtesy of A. L. Mackay; Fig. 19.7 courtesy of J.L. Woods; Fig. 19.10: Tilings were produced using QuasiTiler from the Geometry Center at the University of Minnesota – simulated diffraction patterns courtesy of S. Weber; Fig. 19.14, R. A. Dunlap, M.E. McHenry, R. Chatterjee, and R.C. O'Handley, *Phys. Rev. B* **37**, 8484–7, 1988, Copyright (1988) by the American Physical Society; Fig. 19.17 courtesy of F. Gayle, NIST Gaithersburg; Fig. 19.18 courtesy of W. Ohashi and F. Spaepen; (a) and (b) were originally published in *Nature* (Ohashi and Spaepen, 1987) and (c) appears in the 1989 Harvard Ph.D. thesis of W. Ohashi; Fig. 19.19(a) courtesy of the Materials Research Society, Warrendale, PA; Figure in Box 20.1 courtesy of M. Willard; Fig. 20.6(a) and (b) courtesy of J. Hess and (c) N. Hayward; Fig. 20.16 courtesy of R. Swaminathan; Figure in Box 21.1 courtesy of R. Swaminathan; Figure in Box 22.1 courtesy of M. Hawley, LANL; Fig. 22.6(a) courtesy of S. Chu; Fig. 22.15(a) courtesy of B. Raveau; Fig. 24.1(b) L. Bosio, G. P. Johari, and J. Teixeira, *Phys. Rev. Lett.*, **56**, 460–3, 1986, Copyright (1986) by the American Physical Society; Figure in 24.1 courtesy of M. Bockstaller.

The following figures are new to this edition. Figure 2.10(a) appears on www.chemheritage.org/discover/online-resources/chemistry-in-history/themes/atomic-and-nuclear-structure/rutherford.aspx, and is provided from the Edgar Fahs Smith Memorial Collection, Department of Special Collections, University of Pennsylvania Library. Figure 2.10(b) appears on wikipedia (<http://en.wikipedia.org/wiki/File:Chadwick.jpg>):

photograph by Bortzells Esselte, Nobel Foundation, submitted to wikipedia through the AIP Emilio Segre Visual Archives, Weber and Fermi Film Collections. figure 3.19(c) is courtesy of the Oak Ridge National Laboratory. Figure 11.25(a) is taken from *Les Prix Nobel, En 1913, Stockholm*, Imprimerie Royal. P. A. Norstedt & Soner (frame between page 100 and 101) (1914). Figure 11.25(b) is taken from *Les Prix Nobel, En 1913, Stockholm*, Imprimerie Royal. P. A. Norstedt & Soner (frame between page 102 and 103) (1914). Figure 12.9(a) is reproduced from http://imagine.gsfc.nasa.gov/docs/people/Wilhelm_Roentgen.html. Figure 12.9(b), http://en.wikipedia.org/wiki/File:Max_von_Laue.jpg, comes from *Les Prix Nobel, En 1913, Stockholm*, Imprimerie Royal. P. A. Norstedt & Soner (frame between page 98 and 99) (1914). Figure 13.18(a) is reproduced with permission from the General Photograph Collection, Carnegie Mellon University Archives, Pittsburgh, PA. Figure 15.16(b) is courtesy of Kathleen A. Gallagher. Figure 21.24(b) comes from www.notablebiographies.com/Ni-Pe/Pauling-Linus.html. Figure 22.15(b) is courtesy of IBM Research – Zurich. Figure 24.29(a) comes from R. M Siegel and E. M. Callaway: *Francis Crick's Legacy for Neuroscience: Between the α and the Ω* . PLoS Biol 2/12/2004:e419. <http://dx.doi.org/10.1371/journal.pbio.0020419>. Figure 24.29(b) is courtesy of the Chemical Heritage Foundation Collection.

Symbols

Roman letters			
(H, K, L)	Quasicrystal Miller indices	g	Reciprocal lattice vector
$(n_1n_2n_3n_4)$	Penrose vertex configuration	g_{hkl}	Reciprocal lattice vector
(r, θ, ϕ)	Spherical coordinates	I	Body-centering vector
(u, v, w)	Lattice node coordinates	j	Electrical current density vector
(x, y, z)	Cartesian coordinates	k	Wave vector
ΔE	Energy difference	M	Magnetization vector
Δp_x	Momentum uncertainty	n	Unit normal vector
ΔS	Entropy change	P	General material property
ΔT	Temperature difference	Q	Higher-dimensional scattering vector
Δx	Position uncertainty	r	General position vector
$\hbar$	Normalized Planck constant	S	Poynting vector
$\overline{M_n}$	Number average molecular weight	t	Lattice translation vector
$\overline{M_w}$	Weight average molecular weight	$\mathcal{F}$	General field
$\overline{M}$	Average molecular weight	$\mathcal{G}_m^n$	m-D symmetry group in n-D space
$\overline{r^2}$	Radius of gyration	$\mathcal{O}$	General symmetry operator
$\overline{X_n}$	Degree of polymerization	$\mathcal{P}$	Percentage ionic character
A, B, C	Face-centering vectors	$\mathcal{P}$	Probability
A_i[*], C[*]	Hexagonal reciprocal basis vectors	$\mathcal{R}$	General material response
a, b, c	Bravais lattice basis vectors	$\mathcal{S}(k)$	kth order Fibonacci matrix
a[*], b[*], c[*]	Reciprocal basis vectors	$\mathcal{T}$	Bravais lattice
a_i[*]	Reciprocal basis vectors	$\mathcal{T}$	Plane tiling
a_i	Bravais lattice basis vectors	$\mathcal{W}$	4 × 4 symmetry matrix
C_h	Chiral vector	$\tilde{x}_j$	Normal coordinates
D_i(θ)	Rotation matrix in I-D space	{a, b, γ}	Net parameters
E	Electrical field vector	{a, b, c, α, β, γ}	Lattice parameters
e_i	Cartesian basis vectors	A	Absorption correction factor
e_r	Radial unit vector	A	Atomic weight
F	Interatomic force vector	A	Electron affinity
		a_R	Quasi lattice constant
		a_{ij}	Direct structure matrix
		B(T)	Debye–Waller factor
		B_i	Magnetic induction components

Symbols

b	Neutron scattering length	K	Normalization constant
b_M	Neutron magnetic scattering length	$K, L, M, \dots$	Spectroscopic principal quantum numbers
b_{ij}	Reciprocal structure matrix	k_B	Boltzmann constant
C	Velocity of light in vacuum	L	Potential range
D	Detector	$L(x, y)$	2-D lattice density
D	Distance between two points	L, S	Fibonacci segment lengths
D_i	Electric displacement components	l	Angular momentum quantum number
d_{hkl}	Interplanar spacing	l_i	Direction cosines
E	Electric field strength	L_n	Lucas numbers
E	Electronegativity	$L_p(\theta)$	Lorentz polarization factor
E	Number of polygon edges	M	Debye–Waller factor
E	Photon energy	M_W	Molecular weight
E_i	Electric field components	m	Magnetic quantum number
E_n	Energy levels	m	Particle mass
E_p	Potential energy	m_0	Electron rest mass
E_{kin}	Kinetic energy	m_i	Mass flux components
e	Electron charge	m_n	Neutron rest mass
e_{ijk}^*	Normalized reciprocal per mutation symbol	N_e	Number of free electrons
e_{ijk}	Normalized permutation symbol	n	Principal quantum number
F	Number of polygon faces	n, l, m	Atomic quantum numbers
F_k	Fibonacci numbers	P	Synchrotron total power
F_{hkl}	Structure factor	p	Subgroup index
$f(s)$	Atomic scattering factor	$P(\mathbf{r})$	Patterson function
f^{el}	Electron scattering factor	$P(\theta)$	Polarization factor
G	Optical gyration constant	$p_i, q_i, \dots$	General position vector components
$g(r)$	Pair correlation function	p_{hkl}	Multiplicity of the plane (hkl)
g_{ij}^*	Reciprocal metric tensor	$R_{nl}(r)$	Radial atomic wave function
g_i^*	Reciprocal lattice vector components	R_p	Profile agreement index
g_{ij}	Direct space metric tensor	R_{wp}	Weighted profile agreement index
H_i	Magnetic field components	$RDF(r)$	Radial distribution function
h	Planck’s constant	r	Radial distance
h_i	Heat flux components	r_{ws}	Wigner–Seitz radius
I	Intensity	r_N	Nuclear radius
I	Ionization potential	S	Sample
I_0	Incident beam intensity	s	Scattering parameter
I_{hkl}	Diffacted beam intensity	s	Spin quantum number
$i(k)$	Reduced intensity function	$s, p, d, f, g, \dots$	Spectroscopic angular momentum quantum numbers
J_c	Critical current density	s_i	Planar intercepts
j	Electrical current density	T	Absolute temperature
		T	Target
		T	Triangulation number

T_0	Equal free-energy temperature	ε	Lennard-Jones energy scale parameter
T_c	Superconductor critical temperature	ε_{ijk}^*	Reciprocal permutation symbol
T_g	Glass transition temperature	ε_0	Permittivity of vacuum
T_L	Liquidus temperature	ε_F	Fermi energy level
T_N	Néel temperature	ε_{ijk}	Permutation symbol
T_{rg}	Reduced glass transition temperature	ε_{ij}	Strain tensor
T_{x1}	Primary recrystallization temperature	θ_{hkl}	Bragg angle
T_{x2}	Secondary recrystallization temperature	λ	Photon electron neutron, or radiation wavelength
t	Grain size	μ	Linear absorption coefficient
u_i	Lattice translation vector components	μ/ρ	Mass absorption coefficient
V	Accelerating voltage	ν	Photon frequency
V	Electrostatic potential drop	ν_0	Zero-point motion frequency
V	Number of polygon vertices	ρ	Density
V	Unit cell volume	$\rho(\mathbf{r})$	Charge density
$V(r)$	Radial electrostatic potential	$\rho_{\text{atom}}(r)$	Spatially dependent atomic density
$V_c(r)$	Coulomb interaction potential	σ	Electrical conductivity
$V_r(r)$	Repulsive interaction potential	σ	Scattering cross section
$Y_{lm}(\theta, \phi)$	Angular atomic wave function	σ	Lennard-Jones distance parameter
		σ_{ij}	Electrical conductivity tensor
		σ_{ij}	Stress tensor
		τ	Golden mean
		ϕ	Chiral angle
Z	Atomic number	ϕ	Phase of a wave
a	Anorthic	χ	Mulliken electronegativity
c	Cubic	$\chi(k)$	Absorption function (EXAFS)
h	Hexagonal	$\Psi(\mathbf{r})$	General wave function
m	Monoclinic	Ω	Atomic volume
o	Orthorhombic		
R	Rhombohedral		
t	Tetragonal		
			Special symbols
	Greek letters	(ϕ, ρ)	Stereographical projection coordinates
α	Madelung constant	$(D \mathbf{t})$	Seitz symbol
α_{ij}	General coordinate transformation matrix	(hkl)	Hexagonal Miller–Bravais indices
$\Delta\beta_{ij}$	Change of impermeability tensor	(hkl)	Miller indices of a plane
δ_{ij}	Identity matrix	$[uvw]$	Hexagonal Miller–Bravais direction indices
δ_{ij}	Kronecker delta		

Symbols

$[uvw]$	<i>Direction symbol</i>	$\oplus$	<i>Direct product operator</i>
$\square$	<i>Vacancy</i>	$\mathcal{F}$	<i>Fourier transform operator</i>
$\cdot$	<i>Vector dot product operator</i>	$\rightarrow$	<i>Homomorphism</i>
$\det$	<i>Determinant operator</i>	$\subset$	<i>Group–subgroup</i>
$\exists$	<i>“There exists”</i>		<i>relation symbol</i>
$\forall$	<i>“For all, for each”</i>	$\times$	<i>Vector cross product</i>
$\in$	<i>“Belongs to, in”</i>		<i>operator</i>
$\langle uvw \rangle$	<i>Family of directions</i>	$ \quad $	<i>Norm of a vector</i>
$\leftrightarrow$	<i>Isomorphism</i>	$\{hkl\}$	<i>Family of planes</i>