Structure of Materials

Blending rigorous presentation with ease of reading, this is a self-contained textbook on the fundamentals of crystallography, symmetry, and diffraction. Emphasis is placed on combining visual illustrations of crystal structures with the mathematical theory of crystallography to understand the complexity of a broad range of materials. The first half of the book describes the basics of crystallography, discussing bonding, crystal systems, symmetry, and concepts of diffraction. The second half is more advanced, focusing on different classes of materials, and building on an understanding of the simpler to more complex atomic structures. Geometric principles and computational techniques are introduced, allowing the reader to gain a full appreciation of material structure, including metallic, ceramic, amorphous, molecular solids, and nanomaterials. With over 430 illustrations, 400 homework problems, and structure files available to allow the reader to reconstruct many of the crystal structures shown throughout the text, this is suitable for a one-semester advanced undergraduate or graduate course within materials science and engineering, physics, chemistry, and geology.

Additional resources for this title, including solutions for instructors, data files for crystal structures, and appendices are available at www.cambridge.org/9780521651516.

All crystal structure illustrations in this book were made using CrystalMaker®: a crystal and molecular visualization program for Mac and Windows computers (http://www.crystalmaker.com).

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Structure of Materials: An Introduction to Crystallography, Diffraction, and Symmetry

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in memory of Mary Ann (McHenry) Bialosky (1962–99), 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.

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Frontmatter
More information

Contents

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Preface

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 and improved ideas for those who will struggle afterwards.

The title of this book (*The 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

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

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 the structure of matter. 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 benefitted 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 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 web site, 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 succinctly describe crystal structures. 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 to 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, multimedia 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 web site. 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 web site. Weblinks to all companies are provided through the book's web site.

- **Commercial packages**:
  - Adobe Illustrator [http://www.adobe.com/]
  - Adobe Photoshop [http://www.adobe.com/]
  - CrystalMaker and CrystalDiffract [http://www.crystalmaker.com/]
- **Shareware packages**:
  - QuasiTiler [http://www.geom.uiuc.edu/apps/quasitiler/]
  - Kaleidotile (Version 1.5) [http://geometrygames.org/]
- **Free packages**:
  - teTEX [http://www.tug.org/]
  - TeXShop [http://www.texshop.org/]
  - POVray [http://www.povray.org/]

The web site for this book runs on a dedicated Linux workstation located in MDG's office. The site can be reached through the publisher's web site, or, directly, at the following Uniform Resource Locator:

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 that we have inadvertently forgotten. First of all, we would like to express our sincere gratitude to the many teachers that 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 which 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 continues 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 also has 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 Multimedia 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, 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."

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.

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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 re-write (and, often, re-write again) the various sections of this book.

Michael McHenry would like to acknowledge the support and encouragement of his wife, Theresa, during the many years he has been preoccupied with this text. Her patience and encouragement, in addition to her contributions to keeping hardware and software working in his household during this process, were instrumental in its completion. 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 McHenry's son Michael has developed an interest in computer networking and helped to solve many of a middle-aged (old!) man's 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); 3.15(a); 4.4(a),(b); 5.11(a),(b); 6.4(a),(b); 7.12(a),(b); 8.20(a),(b); 9.15(b); 10.13(a),(b); 15.15(a); 16.18(a),(b); 19.25(a); 20.19(b); 21.18(a),(b); 22.23(a); 24.23(a),(b).

The following figures were obtained from the Nobel museum and are reproduced with permission: 2.10(a),(b); 3.15(b); 11.25(a),(b); 12.9(a),(b); 13.18(a),(b); 15.15(b); 22.23(b); 23.19(b); 25.28(a),(b);

The 1913 article by W. L. and W. H. Bragg on the structure determination of diamond (historical notes in Chapter 14, W. H. Bragg and W. L. Bragg (The Structure of the Diamond) *Proc. R. Soc. A*, **89**, pp. 277–291 (1913)) was reproduced with permission from The Royal Society.

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; 8.15; 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. 1.5 courtesy of P. Ohodnicki; 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 16.6 courtesy of M. Skowronski; Figure in Box 17.6 courtesy of M. Tanase, D. E. Laughlin and J.-G. Zhu; Figure in Box 17.9 courtesy of K. Barmak; Fig. 17.29(a) courtesy of Department of Materials, University of Oxford; Fig. 17.29(b) courtesy of T. Massalski; Figure in Box 18.4 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; Figure in Box 19.1 courtesy of E. Shevshenko

and Chris Murray, IBM; Fig. 19.25(b) courtesy of C. Shoemaker; Fig. 20.10: Tilings were produced using QuasiTiler from the Geometry Center at the University of Minnesota – simulated diffraction patterns courtesy of S. Weber; Fig. 20.7 courtesy of J. L. Woods; Fig. 20.14, R. A. Dunlap, M. E. McHenry, R. Chaterjee, and R. C. O'Handley, Phys. Rev. B **37**, 8484–7, 1988, Copyright (1988) by the American Physical Society; Fig. 20.17 courtesy of F. Gayle, NIST Gaithersburg; Fig. 20.18 courtesy of W. Ohashi and F. Spaepen; (a) and (b) were originally published in Nature (Ohashi and Spaepen, 1987) and (c) appears in the Harvard Ph.D. thesis of W. Ohashi; Fig. 20.19(a) courtesy of the Materials Research Society, Warrendale, PA; Figure in Box 21.1 courtesy of M. Willard; Fig. 21.6(a) and (b) courtesy of J. Hess and (c) N. Hayward; Fig. 21.16 courtesy of R. Swaminathan; Figure in Box 22.7 courtesy of R. Swaminathan; Figure in Box 23.4 courtesy of M. Hawley, LANL; Fig. 23.8(a) courtesy of S. Chu; Fig. 23.19(a) courtesy of B. Raveau; Fig. 25.1(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 Box 25.5 courtesy of M. Bockstaller.

Atomic coordinates of known higher fullerenes have been graciously made available at the website of Dr. M. Yoshida; http://www.cochem2.tutkie.tut.ac.jp/Fuller/Fuller.html.

Symbols

	Roman letters
(H, K, L)	*Quasicrystal Miller indices*
$(n_1 n_2 n_3 n_4)$	*Penrose vertex configuration*
(u, v, w)	*Lattice node coordinates*
(x, y, z)	*Cartesian coordinates*
ΔE	*Energy difference*
Δp_x	*Momentum uncertainty*
ΔS	*Entropy change*
ΔT	*Temperature difference*
Δx	*Position uncertainty*
$\hbar$	*Normalized Planck constant*
$\mathbf{A}_i^*, \mathbf{C}^*$	*Hexagonal reciprocal basis vectors*
c	*Velocity of light in vacuum*
$\mathbf{D}_i(\theta)$	*Rotation matrix in i-dimensional space*
ν	*Frequency of an electromagnetic wave*
$\overline{M_\mathrm{n}}$	*Number average molecular weight*
$\overline{M_\mathrm{w}}$	*Weight average molecular weight*
$\overline{M}$	*Average molecular weight*
$\overline{r^2}$	*Radius of gyration*
$\overline{X_n}$	*Degree of polymerization*
$\mathcal{T}$	*Plane tiling*
$\mathbf{A}, \mathbf{B}, \mathbf{C}$	*Face centering vectors*
$\mathbf{a}, \mathbf{b}, \mathbf{c}$	*Bravais lattice basis vectors*
$\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$	*Reciprocal basis vectors*
$\mathbf{a}_i^*$	*Reciprocal basis vectors*
$\mathbf{a}_i$	*Bravais lattice basis vectors*
$\mathbf{C}_h$	*Chiral vector*
$\mathbf{E}$	*Electrical field vector*
$\mathbf{e}_i$	*Cartesian basis vectors*
$\mathbf{e}_r$	*Radial unit vector*
$\mathbf{F}$	*Interatomic force vector*
$\mathbf{g}$	*Reciprocal lattice vector*
$\mathbf{g}_{hkl}$	*Reciprocal lattice vector*
$\mathbf{I}$	*Body centering vector*
$\mathbf{j}$	*Electrical current density vector*
$\mathbf{k}$	*Wave vector*
$\mathbf{M}$	*Magnetization vector*
$\mathbf{n}$	*Unit normal vector*
$\mathbf{P}$	*General material property*
$\mathbf{Q}$	*Higher-dimensional scattering vector*
$\mathbf{r}$	*General position vector*
$\mathbf{S}$	*Poynting vector*
$\mathbf{t}$	*Lattice translation vector*
$\mathcal{F}$	*General field*
$\mathcal{G}_m^n$	*m-D symmetry group in n-D space*
$\mathcal{P}$	*Percentage ionic character*
$\mathcal{P}$	*Probability*
$\mathcal{R}$	*General material response*
$\mathcal{S}(k)$	*k-th order Fibonacci matrix*
$\mathcal{T}$	*Bravais lattice*
$\mathcal{W}$	4×4 *symmetry matrix*

$\mathcal{O}$	*General symmetry operator*	g_i^*	*Reciprocal lattice vector components*
σ	*Lennard-Jones distance parameter*	g_{ij}	*Direct space metric tensor*
$\mathrm{RDF}(r)$	*Radial distribution function*	h	*Planck's constant*
$\tilde{x}_j$	*Normal coordinates*	H_i	*Magnetic field components*
$\{a, b, \gamma\}$	*Net parameters*	h_i	*Heat flux components*
$\{a, b, c, \alpha, \beta, \gamma\}$	*Lattice parameters*	$H_{c1}(T)$	*Lower critical field*
A	*Absorption correction factor*	$H_{c2}(T)$	*Upper critical field*
A	*Atomic weight*	I	*Intensity*
A	*Electron affinity*	I	*Ionization potential*
a_R	*Quasicrystal lattice constant*	$i(k)$	*Reduced intensity function*
a_{ij}	*Direct structure matrix*	I_0	*Incident beam intensity*
b	*Neutron scattering length*	I_{hkl}	*Diffracted beam intensity*
$B(T)$	*Debye–Waller factor*	j	*Electrical current density*
B_i	*Magnetic induction components*	J_c	*Critical current density*
		K	*Normalization constant*
b_M	*Neutron magnetic scattering length*	K, L, M, . . .	*Spectroscopic principal quantum numbers*
b_{ij}	*Reciprocal structure matrix*	k_B	*Boltzmann constant*
D	*Detector*	L	*Potential range*
D	*Distance between two points*	l	*Angular momentum quantum number*
D_i	*Electric displacement components*	$L(x, y)$	*2-D lattice density*
d_{hkl}	*Interplanar spacing*	L, S	*Fibonacci segment lengths*
E	*Electric field strength*	l_i	*Direction cosines*
E	*Electronegativity*	L_n	*Lucas numbers*
E	*Number of polygon edges*	$L_p(\theta)$	*Lorentz polarization factor*
E	*Photon energy*	M	*Debye–Waller factor*
e	*Electron charge*	m	*Magnetic quantum number*
E_i	*Electric field components*	m	*Particle mass*
E_n	*Energy levels*	m_0	*Electron rest mass*
E_p	*Potential energy*	m_i	*Mass flux components*
E_{kin}	*Kinetic energy*	m_n	*Neutron rest mass*
F	*Number of polygon faces*	M_W	*Molecular weight*
$f(s)$	*Atomic scattering factor*	n	*Principal quantum number*
f^{el}	*Electron scattering factor*	n, l, m	*Atomic quantum numbers*
F_k	*Fibonacci numbers*	N_e	*Number of free electrons*
		P	*Synchrotron total power*
F_{hkl}	*Structure factor*	p	*Subgroup index*
G	*Optical gyration constant*	$P(\mathbf{r})$	*Patterson function*
$g(r)$	*Pair correlation function*	$P(\theta)$	*Polarisation factor*
g_{ij}^*	*Reciprocal metric tensor*		

$p_i, q_i, \ldots$	*General position vector components*
p_{hkl}	*Multiplicity of the plane (hkl)*
r	*Radial distance*
r_N	*Nuclear radius*
R_p	*Profile agreement index*
r_ws	*Wigner–Seitz radius*
$R_{nl}(r)$	*Radial atomic wave function*
R_wp	*Weighted profile agreement index*
S	*Sample*
s	*Scattering parameter*
s	*Spin quantum number*
$s, p, d, f, g, \ldots$	*Spectroscopic angular momentum quantum numbers*
s_i	*Planar intercepts*
T	*Absolute temperature*
T	*Target*
T	*Triangulation number*
t	*Grain size*
T_0	*Equal free-energy temperature*
T_c	*Superconductor critical temperature*
T_g	*Glass transition temperature*
T_L	*Liquidus temperature*
T_N	*Nëel temperature*
T_rg	*Reduced glass transition temperature*
T_{x1}	*Primary recrystallization temperature*
T_{x2}	*Secondary recrystallization temperature*
u_i	*Lattice translation vector components*
V	*Accelerating voltage*
V	*Electrostatic potential drop*
V	*Number of polygon vertices*
V	*Unit cell volume*
$V(r)$	*Radial electrostatic potential*
$V_\mathrm{c}(r)$	*Coulomb interaction potential*
$V_\mathrm{r}(r)$	*Repulsive interaction potential*
$Y_{lm}(\theta, \phi)$	*Angular atomic wave function*
Z	*Atomic number*
a	*Anorthic*
c	*Cubic*
h	*Hexagonal*
m	*Monoclinic*
o	*Orthorhombic*
R	*Rhombohedral*
t	*Tetragonal*

Greek letters

(r, θ, ϕ)	*Spherical coordinates*
α	*Madelung constant*
α_{ij}	*General coordinate transformation matrix*
χ	*Mulliken electronegativity*
$\chi(k)$	*Absorption function (EXAFS)*
$\Delta\beta_{ij}$	*Change of impermeability tensor*
δ_{ij}	*Identity matrix*
δ_{ij}	*Kronecker delta*
ϵ	*Lennard-Jones energy scale parameter*
ϵ^*_{ijk}	*Reciprocal permutation symbol*
ϵ_0	*Permittivity of vacuum*
ϵ_F	*Fermi energy level*
ϵ_{ijk}	*Permutation symbol*
ϵ_{ij}	*Strain tensor*
λ	*Photon/electron/neutron wave length*
λ	*radiation wave length*
μ	*Linear absorption coefficient*

μ/ρ	*Mass absorption coefficient*	$(\mathrm{D}\|\mathbf{t})$	*Seitz symbol*
ν	*Photon frequency*	$(hkil)$	*Hexagonal Miller–Bravais indices*
ν_0	*Zero-point motion frequency*		
Ω	*Atomic volume*	(hkl)	*Miller indices of a plane*
ϕ	*Chiral angle*	$[uvtw]$	*Hexagonal Miller–Bravais direction indices*
ϕ	*Phase of a wave*		
$\Psi(\mathbf{r})$	*General wave function*	$[uvw]$	*Direction symbol*
ρ	*Density*	$\square$	*Vacancy*
$\rho(\mathbf{r})$	*Charge density*	$\cdot$	*Vector dot product operator*
$\rho_{\mathrm{atom}}(r)$	*Spatially dependent atomic density*	det	*Determinant operator*
		$\exists$	*"there exists"*
σ	*Electrical conductivity*	$\forall$	*"for all, for each"*
σ	*Scattering cross section*	$\in$	*"belongs to, in"*
σ_{ij}	*Electrical conductivity tensor*	$\langle uvw\rangle$	*Family of directions*
		$\leftrightarrow$	*Isomorphism*
σ_{ij}	*Stress tensor*	$\oplus$	*Direct product operator*
τ	*Golden mean*	$\mathcal{F}$	*Fourier transform operator*
θ_{hkl}	*Bragg angle*	$\rightarrow$	*Homomorphism*
e^*_{ijk}	*Normalized reciprocal permutation symbol*	$\subset$	*group–subgroup relation symbol*
e_{ijk}	*Normalized permutation symbol*	$\times$	*Vector cross product operator*
	Special symbols	$\|\ \|$	*Norm of a vector*
(ϕ, ρ)	*Stereographical projection coordinates*	$\{hkl\}$	*Family of planes*