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

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/degraef).

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

Structure of Materials

AN INTRODUCTION TO CRYSTALLOGRAPHY, DIFFRACTION AND SYMMETRY

MARC DE GRAEF
Carnegie Mellon University, Pittsburg

MICHAEL E. McHENRY
Carnegie Mellon University, Pittsburg

Second edition, fully revised and updated

CAMBRIDGE
UNIVERSITY PRESS

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

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
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.

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

Contents

CAMBRIDGE
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
978-1-107-00587-7 — Structure of Materials
2nd Edition
Marc De Graef , Michael E. McHenry
Frontmatter
More Information

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
978-1-107-00587-7 — Structure of Materials
2nd Edition
Marc De Graef , Michael E. McHenry
Frontmatter
More Information

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

Contents

Contents

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

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.

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

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.crystalmaker.com].

- **Shareware packages**:
  - QuasiTiler [www.geom.uiuc.edu/apps/quasitiler];
  - Kaleidotile (Version 1.5) [http://geometrygames.org].
- **Free packages**:
  - teTEX [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, 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. Chaterjee, 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/onlune-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.jpj):

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*. PLiS Biol 2/12/2004:e419. http://dx.doi.org/10.1371.jopurnal.pbio.0020419. Figure 24.29(b) is courtesy of the Chemical Heritage Foundation Collection.

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

Symbols

Roman letters

(H, K, L)	*Quasicrystal Miller indices*
$(n_1 n_2 n_3 n_4)$	*Penrose vertex configuration*
(r, θ, ϕ)	*Spherical coordinates*
(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*
$\overline{M}_\mathrm{n}$	*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*
$\mathbf{A}, \mathbf{B}, \mathbf{C}$	*Face-centering vectors*
$\mathbf{A}_i^*, \mathbf{C}^*$	*Hexagonal reciprocal basis 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*
$\mathbf{D}_i(\theta)$	*Rotation matrix in* I-D *space*
$\mathbf{E}$	*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*
$\mathscr{F}$	*General field*
$\mathscr{G}_m^n$	*m-D symmetry group in n-D space*
$\mathscr{O}$	*General symmetry operator*
$\mathscr{P}$	*Percentage ionic character*
$\mathscr{P}$	*Probability*
$\mathscr{R}$	*General material response*
$\mathscr{S}(k)$	*kth order Fibonacci matrix*
$\mathscr{T}$	*Bravais lattice*
$\mathscr{T}$	*Plane tiling*
$\mathscr{W}$	*4 × 4 symmetry matrix*
$\tilde{x}_j$	*Normal coordinates*
$\{a, b, \gamma\}$	*Net parameters*
$\{a, b, c, \alpha, \beta, \gamma\}$	*Lattice parameters*
A	*Absorption correction factor*
A	*Atomic weight*
A	*Electron affinity*
a_R	*Quasi lattice constant*
a_{ij}	*Direct structure matrix*
$B(T)$	*Debye–Waller factor*
B_i	*Magnetic induction components*

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

b	*Neutron scattering length*	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*
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*	$L_{\mathrm{p}}(\theta)$	*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 permutation 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*	$p_i, q_i, \ldots$	*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*	$\mathrm{RDF}(r)$	*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}	*Diffracted beam intensity*	s	*Spin quantum number*
$i(k)$	*Reduced intensity function*	$s, p, d, f, g, \ldots$	*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*

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

T_0	*Equal free-energy temperature*
T_c	*Superconductor critical temperature*
T_g	*Glass transition temperature*
T_L	*Liquidus temperature*
T_N	*Néel temperature*
T_{rg}	*Reduced glass transition temperature*
T_{x1}	*Primary recrystallization temperature*
T_{x2}	*Secondary recrystallization temperature*
t	*Grain size*
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*
$V_c(r)$	*Coulomb interaction potential*
$V_r(r)$	*Repulsive interaction potential*
$Y_{lm}(\theta, \phi)$	*Angular atomic wave function*

Subscripts

Z	*Atomic number*
a	*Anorthic*
c	*Cubic*
h	*Hexagonal*
m	*Monoclinic*
o	*Orthorhombic*
R	*Rhombohedral*
t	*Tetragonal*

Greek letters

α	*Madelung constant*
α_{ij}	*General coordinate transfor mation matrix*
$\Delta\beta_{ij}$	*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*
θ_{hkl}	*Bragg angle*
λ	*Photon electron neutron, or radiation wavelength*
μ	*Linear absorption coefficient*
μ/ρ	*Mass absorption coefficient*
ν	*Photon frequency*
ν_0	*Zero-point motion frequency*
ρ	*Density*
$\rho(\mathbf{r})$	*Charge density*
$\rho_{atom}(r)$	*Spatially dependent atomic density*
σ	*Electrical conductivity*
σ	*Scattering cross section*
σ	*Lennard-Jones distance parameter*
σ_{ij}	*Electrical conductivity tensor*
σ_{ij}	*Stress tensor*
τ	*Golden mean*
ϕ	*Chiral angle*
ϕ	*Phase of a wave*
χ	*Mulliken electronegativity*
$\chi(k)$	*Absorption function (EXAFS)*
$\Psi(\mathbf{r})$	*General wave function*
Ω	*Atomic volume*

Special symbols

(ϕ, ρ)	*Stereographical projection coordinates*
$(\mathrm{D}\|\mathbf{t})$	*Seitz symbol*
$(hkil)$	*Hexagonal Miller–Bravais indices*
(hkl)	*Miller indices of a plane*
$[uvtw]$	*Hexagonal Miller–Bravais direction indices*

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

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