Structure and Bonding in Crystalline Materials

One of the motivating questions in materials research today is: how can elements be combined to produce a solid with specified properties? One part of the answer to this question lies in the fundamental relationship between the composition, structure and bonding in crystalline materials. This book is intended to acquaint the reader with established principles of crystallography and bonding that are needed to understand this relationship.

The book starts with an introduction to periodic trends and then describes the atomic structure of crystalline solids, the experimental interrogation of crystalline structure, the origin of the cohesive forces that stabilize crystalline structures, and how these cohesive forces vary with the elements in the solid. The book finishes by describing a number of models for predicting phase stability and structure.

Containing a large number of worked examples, exercises, and detailed descriptions of numerous crystal structures, this book is primarily intended as an advanced undergraduate or graduate level textbook for students of materials science who are preparing to conduct research. However, it will also be useful to scientists and engineers who work with solid materials.

GREGORY S. ROHRER is a Professor of Materials Science and Engineering at Carnegie Mellon University. Prof. Rohrer was born in Lancaster, PA, in 1962. He received his bachelor's degree in Physics from Franklin and Marshall College in 1984 and his Ph.D. in Materials Science and Engineering from the University of Pennsylvania in 1989. At CMU, Prof. Rohrer is the director of the NSF sponsored Materials Research Science and Engineering Center. His research is directed toward understanding how the properties of surfaces and internal interfaces are influenced by their geometric and crystallographic structure, their stoichiometry, and their defect structure. Prof. Rohrer is an associate Editor for the Journal of the American Ceramic Society and his research earned a National Science Foundation Young Investigator Award in 1994.

Structure and Bonding in Crystalline Materials

GREGORY S. ROHRER

CAMBRIDGE
UNIVERSITY PRESS

PUBLISHED BY THE PRESS SYNDICATE OF THE UNIVERSITY OF CAMBRIDGE
The Pitt Building, Trumpington Street, Cambridge, United Kingdom

CAMBRIDGE UNIVERSITY PRESS
The Edinburgh Building, Cambridge CB2 2RU, UK
40 West 20th Street, New York, NY 10011–4211, USA
10 Stamford Road, Oakleigh, VIC 3166, Australia
Ruiz de Alarcón 13, 28014 Madrid, Spain
Dock House, The Waterfront, Cape Town 8001, South Africa

http://www.cambridge.org

First published 2001

Printed in the United Kingdom at the University Press, Cambridge

Typeset in Times NR MT 10/13pt, in QuarkXPress™ [SE]

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

ISBN 0 521 66328 8 hardback
ISBN 0 521 66379 2 paperback

Contents

Preface

This book resulted from lecture notes that I compiled while teaching a course of the same name in the Department of Materials Science and Engineering at Carnegie Mellon University. When I began teaching this class in the early 1990s, there were already excellent textbooks on crystallography, solid state physics, and structural solid state chemistry. However, none of these books by themselves were entirely appropriate for the course I intended to teach to graduate students in materials science and engineering. Therefore, I have attempted to combine the subject matter in a way that would be both appealing and useful for materials scientists and engineers. Included in the book are compilations of data that are a useful resource for students and researchers considering basic structural problems. Much of the material in the book is derived from secondary sources and, to the best of my ability, I have assigned credit to these books in the last section of each chapter, under 'References and Sources for Further Study'. Books by Burger (Contemporary Crystallography), Sands (Introduction to Crystallography), Harrison (Electron Structure and the Properties of Solids), West (Solid State Chemistry and its Applications), Wells (Structural Inorganic Chemistry), Kittel (Introduction to Solid State Physics), and Ashcroft and Mermin (Solid State Physics) were especially useful and it is appropriate that I draw attention to them at the outset.

At Carnegie Mellon University, this course is taught during a 14 week semester consisting of approximately 52 hours of lecture. However, by prioritizing material according to the goals of an individual class, it should be possible to use this book as the basis for abbreviated courses.

This book is the outcome of a National Science Foundation Grant. Specifically, the development of this book was the educational component of a Young Investigator Award (DMR-9458005) that supported my research and educational activities for five years. Assistance also came from the more than 200 students who have been enrolled in my course over the years. The students continually helped me refine the text by pointing out errors and ambiguities. Dr Matt Willard deserves special mention for providing me with extensive detailed comments on an early draft while studying for his Ph.D. qualifying exam. Several other students who worked with me at CMU (Prof. Richard L. Smith, Dr Jennifer B. Lowekamp, and David M. Saylor) contributed figures for this book. My wife, Dr C. Lane Rohrer, was the greatest sustained source of editorial comment. Cathy edited numerous drafts of this book and even contributed several of the sections

where my knowledge was inadequate. While the input I received from Cathy and others has made this a better book, I remain responsible for its deficiencies and any errors that might remain. Finally, I thank my father, C.E. Rohrer, who initially inspired my career in science and to whom I dedicate this book.

G.S. Rohrer
Pittsburgh
February, 2001