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Handbook of Crystallography

For Electron Microscopists and Others

With 114 Figures

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Dedicated
to Gene, whose dream was cut short,
to Alice, who found new dreams,
to Drew, who faced death and chose life.

Preface

This book resulted from a series of frustrations. Analytical electron microscopy requires exactly what its name implies: quantitative information to conduct an analysis. The frustrations arose when I started hunting for specific forms of equations in a form understandable to a non-crystallographer, for definitions of subtle concepts related to crystallography, for intelligible interpretations of space group symbols and their significance. What I frequently discovered was that such information was buried in a giant tome and couched in terms familiar to crystallographers but not to electron microscopists in general, or it was located in an old reference not available in my library, or it was found in an out-of-print book, or it was in a Russian book no longer available, etc.

So to minimize the frustrations, I started a notebook containing the details, particularly after I had found forms of equations useful for quick calculations or equations in a form useful for proving, doing, or extending calculations found in a reference. The resulting notebook grew to a respectable size, requiring some organizing of the contents. Finally, the size became large enough, and has proven useful enough, to produce the notebook as a book.

The readers to whom this book is aimed are those microscopists, and others, who are not crystallographers, but who need details about crystal structures in order to interpret images and diffraction effects and patterns present in the electron microscope. Hence, this book is practically oriented. No attempt has been made to make equations mathematically rigorous beyond the rigor needed to accomplish a calculation. Every attempt has been made to insure the mathematical correctness of the equations, because I found correcting mistakes was a major frustration when using an expression from a reference.

This book is not a handbook of electron microscopy. It is a handbook to be used when doing electron microscopy for which crystallographic information plays a fundamental role in the interpretation of the data and images generated. As a minimum my hope is that the book will be a helpful starting reference source for microscopists, since full treatments of the subjects presented would take considerably more pages than I have devoted to them.

The book is divided into 13 chapters. Although the division is somewhat arbitrary, I have grouped items and subjects where possible. Chapter 1 contains mathematics useful in understanding structures, lattices, and the like. Chapter 2 contains specifics for several common crystal systems, bringing together several definitions to be found in the literature. The purpose here is to highlight the fact that different authors use different definitions, which sometimes are not equivalent or are so specialized that their use beyond the one application leaves a reader stranded. Chapter 3 is a brief overview of diffraction pattern analysis. Chapter 4 covers packing and stacking, one of those subjects that lends itself to misinterpretation because of loose use of symbols, particularly the A, B, C site symbols. Chapter 5 describes the seven crystal systems in detail. This chapter contains the equations for each system that one may need to do simple calculations or to refresh one's memory

about axes used. Chapter 6 covers transformations of crystal system axes in a practical way. Chapter 7 deals with slip systems. Chapter 8 includes discussions of various projections found to be useful in transmission electron microscopy (TEM). Chapter 9 covers the essentials of symmetry and the wondrous symbolism used in this powerful representation of lattices and structures. Chapter 10 is a brief discussion of convergent beam electron diffraction, especially the use of higher order Laue zone (holz) rings and the parities of the rings. Chapter 11 contains miscellaneous tables that I have found of some value. Chapter 12 is an introduction to icosahedral symmetry and diffraction patterns. The last chapter contains the essentials about dislocations and has tables useful for simple contrast analysis.

Although the list of references is far from complete, they include all those I have found to contain data useful for my needs and in extending my understanding of the fundamental principles underlying crystallography and structures. Of those listed, the following are recommended as good places to go when questions arise:

Barrett , C. S. and T. B Massalski, *Structure of Metals,* Pergamon Press, New York, 1980.
Brown, P. J. and J. B. Forsyth, *The Crystal Structure of Solids,* Edward Arnold Ltd, London, 1979.
Deer, W. A., R. A. Howie, and J. Zussman, *An Introduction to the Rock-Forming Minerals*, Longman Group, Ltd., London, 1980 [available through Halsted Press, Division of John Wiley & Sons, Inc., New York].
Pearson, W. B., *The Crystal Chemistry and Physics of Metals and Alloys*, Wiley- Interscience, New York, 1972.
Vainstein, B. K., A. A. Chernov and L. A. Shuvalov (editors), *Modern Crystallography*, Volumes I-IV, Springer-Verlag, New York, 1979.

It is a pleasure to acknowledge the help and assistance of a number of people. My thanks to Judy Paine for hunting for books in the library when I had given up, to Jeffrey Robbins for his encouragement, to Tom Broderick for helpful discussions concerning slip, to Karen Teal for her encouragement, to Materials Laboratory, and to Systems Research Laboratories for permission to publish, to Dr. C. Suryanarayana for helpful suggestions concerning icosahedral symmetry and comments on the contents, and to my students who have offered suggestions and pointed out errors. I am particularly grateful to the University of Dayton Department of Materials Science for the opportunities to teach from 1984 to 1990. I thank Dr. Dan Miracle for permission to use in Chapter 10 the extended form of the table on diffraction symbols and point groups prior to publication. My thanks also to the production and editorial staff at Springer-Verlag for their constructive suggestions and help.

The following have given permissions to use examples and figures from publications: The Royal Society of London, John Wiley and Sons, ASM International, and the American Physical Society.

Preparation of any book is inevitably a family affair. Hence, my thanks to my spouse, Marti, who played a major role by her expressions of interest and her help in reviewing the early manuscripts, to my daughter, Michelle, for proofing several sections for me, and to my son, Mike, for giving up his tennis table for months.

Any errors present are my responsibility. There are subjects of importance that I have not included, such as matrix representations of symmetry operations, disclinations, and ceramic structures related to minerals. My apologies for such omissions, but the references provided are good starting points for finding more information on these subjects. I will appreciate any comments, thoughts, and suggestions readers may have, complimentary or otherwise.

Preparation of the manuscript was accomplished using the Microsoft Word program on the Macintosh SE. Equations were prepared using the mathematics typesetting codes in Word. Figures were prepared using CricketDraw. The original text was printed on Laserprint paper using a Laserprinter II NT.

Dayton, Ohio
January, 1991

A. G. Jackson

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Definitions and Mathematics

1.1. Definitions

crystal ≡ a material in which the atoms are arranged in a translationally periodic array in three dimensions or which are arranged in rotationally periodic arrays in three dimensions [Cullity , 1978].

lattice ≡ array of points in three-dimensional space; each point displays identical symmetry.

crystallographic point ≡ a point in a lattice that displays the symmetry of the lattice. The crystallographic point is not the same as a mathematical point, which has zero dimensions and has no symmetry associated with it [Vainstein, 1979].

unit cell ≡ a volume characterized by vectors **a,b,c** which are taken from a common origin and are all not coplanar. Repetition of this cell generates the lattice.

$\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ ≡ alternate notation for axes **a**, **b**, **c.**

crystallographic axes ≡ **a, b, c** of the unit cell.

lattice constant(s) ≡ lattice parameters; the repeat distances along each of the crystallographic axes; magnitudes of the vectors **a, b, c**, and angles between axes.

basis vectors ≡ unit vectors in terms of which **a, b, c** are defined.

orthogonal basis ≡ set of vectors that satisfy $\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$.

basis ≡ motif ≡ group of atoms associated with a lattice point.

primitive cell ≡ **simple cell** ≡ **P** ≡ lattice unit cell with one lattice point per cell, or the minimum number of points possible in the lattice unit cell.

Laue class ≡ symbol expressing the point symmetry of the crystal system as observed in the diffraction pattern; the symmetry of the reciprocal lattice times the intensity of the (hkl) plane.

Laue zone ≡ those reciprocal lattice points that lie in planes parallel to the first reciprocal lattice plane that intercepts the Ewald sphere; $\mathbf{g} \cdot \mathbf{u} = N$, where **g** = reciprocal lattice vector, **u** = direction vector defining the diffraction zone axis, N = integer = number of the Laue zone.

zone axis ≡ the axis formed by those reciprocal lattice vectors which satisfy $\mathbf{g} \cdot \mathbf{u} = 0$; the axis is parallel to the direction vector **u**.

1.2. Vector Operations

1.2.1. Dot and cross products

For a triad of vector axes (**a**, **b**, **c**) defined in terms of an orthonormal reference coordinate system ($\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$), the two most frequently used vector operations in electron diffraction crystallography) are :

Dot product **a** • **b**, where