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ELEMENTS OF X-RAY DIFFRACTION

by

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ADDISON-WESLEY PUBLISHING COMPANY, Inc.

READING, MASSACHUSETTS

Printed in the United States of America

Library of Congress Catalog No. 56-10137

PREFACE

X-ray diffraction is a tool for the investigation of the fine structure of matter. This technique had its beginnings in von Laue's discovery in 1912 that crystals diffract x-rays, the manner of the diffraction revealing the structure of the crystal. At first, x-ray diffraction was used only for the determination of crystal structure. Later on, however, other uses were developed, and today the method is applied, not only to structure determination, but to such diverse problems as chemical analysis and stress measurement, to the study of phase equilibria and the measurement of particle size, to the determination of the orientation of one crystal or the ensemble of orientations in a polycrystalline aggregate.

The purpose of this book is to acquaint the reader who has no previous knowledge of the subject with the theory of x-ray diffraction, the experimental methods involved, and the main applications. Because the author is a metallurgist, the majority of these applications are described in terms of metals and alloys. However, little or no modification of experimental method is required for the examination of nonmetallic materials, inasmuch as the physical principles involved do not depend on the material investigated. This book should therefore be useful to metallurgists, chemists, physicists, ceramists, mineralogists, etc., namely, to all who use x-ray diffraction purely as a laboratory tool for the sort of problems already mentioned.

Members of this group, unlike x-ray crystallographers, are not normally concerned with the determination of complex crystal structures. For this reason the rotating-crystal method and space-group theory, the two chief tools in the solution of such structures, are described only briefly.

This is a book of principles and methods intended for the student, and not a reference book for the advanced research worker. Thus no metallurgical data are given beyond those necessary to illustrate the diffraction methods involved. For example, the theory and practice of determining preferred orientation are treated in detail, but the reasons for preferred orientation, the conditions affecting its development, and actual orientations found in specific metals and alloys are not described, because these topics are adequately covered in existing books. In short, x-ray diffraction is stressed rather than metallurgy.

The book is divided into three main parts: fundamentals, experimental methods, and applications. The subject of crystal structure is approached through, and based on, the concept of the point lattice (Bravais lattice), because the point lattice of a substance is so closely related to its diffraction pattern. The entire book is written in terms of the Bragg law and can be read without any knowledge of the reciprocal lattice. (However, a brief treatment of reciprocal-lattice theory is given in an appendix for those who wish to pursue the subject further.) The methods of calculating the intensities of diffracted beams are introduced early in the book and used throughout. Since a rigorous derivation of many of the equations for diffracted intensity is too lengthy and complex a matter for a book of this kind, I have preferred a semiquantitative approach which, although it does not furnish a rigorous proof of the final result, at least makes it physically reasonable. This preference is based on my conviction that it is better for a student to grasp the physical reality behind a mathematical equation than to be able to glibly reproduce an involved mathematical derivation of whose physical meaning he is only dimly aware.

Chapters on chemical analysis by diffraction and fluorescence have been included because of the present industrial importance of these analytical methods. In Chapter 7 the diffractometer, the newest instrument for diffraction experiments, is described in some detail; here the material on the various kinds of counters and their associated circuits should be useful, not only to those engaged in diffraction work, but also to those working with radioactive tracers or similar substances who wish to know how their measuring instruments operate.

Each chapter includes a set of problems. Many of these have been chosen to amplify and extend particular topics discussed in the text, and as such they form an integral part of the book.

Chapter 18 contains an annotated list of books suitable for further study. The reader should become familiar with at least a few of these, as he progresses through this book, in order that he may know where to turn for additional information.

Like any author of a technical book, I am greatly indebted to previous writers on this and allied subjects. I must also acknowledge my gratitude to two of my former teachers at the Massachusetts Institute of Technology, Professor B. E. Warren and Professor John T. Norton: they will find many an echo of their own lectures in these pages. Professor Warren has kindly allowed me to use many problems of his devising, and the advice and encouragement of Professor Norton has been invaluable. My colleague at Notre Dame, Professor G. C. Kuczynski, has read the entire book as it was written, and his constructive criticisms have been most helpful. I would also like to thank the following, each of whom has read one or more chapters and offered valuable suggestions: Paul A. Beck, Herbert Friedman, S. S. Hsu, Lawrence Lee, Walter C. Miller, William Parrish, Howard Pickett, and Bernard Waldman. I am also indebted to C. G. Dunn for the loan of illustrative material and to many graduate students, August

Freda in particular, who have helped with the preparation of diffraction patterns. Finally but not perfunctorily, I wish to thank Miss Rose Kunkle for her patience and diligence in preparing the typed manuscript.

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Notre Dame, Indiana
March, 1956

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