

# Preface

X-ray diffraction crystallography for powder samples is well-established and widely used in the field of materials characterization to obtain information on the atomic scale structure of various substances in a variety of states. Of course, there have been numerous advances in this field, since the discovery of X-ray diffraction from crystals in 1912 by Max von Laue and in 1913 by W.L. Bragg and W.H. Bragg. The origin of crystallography is traced to the study for the external appearance of natural minerals and a large amount of data have been systematized by applying geometry and group theory. Then, crystallography becomes a valuable method for the general consideration of how crystals can be built from small units, corresponding to the infinite repetition of identical structural units in space.

Many excellent and exhaustive books on X-ray diffraction and crystallography are available, but the undergraduate students and young researchers and engineers who wish to become acquainted with this subject frequently find them overwhelming. They find it difficult to identify and understand the essential points in the limited time available to them, particularly on how to estimate useful structural information from the X-ray diffraction data. Since X-ray powder diffraction is one of the most common and leading methods in materials research, mastery of the subject is essential.

In order to learn the fundamentals of X-ray diffraction crystallography well and to be able to cope with the subject appropriately, a certain number of “exercises” involving calculation of specific properties from measurements are strongly recommended. This is particularly true for beginners of X-ray diffraction crystallography. Recent general purpose X-ray diffraction equipments have a lot of inbuilt automation for structural analysis. When a sample is set in the machine and the preset button is pressed, results are automatically generated some of which are misleading. A good understanding of fundamentals helps one to recognize misleading output.

During the preparation of this book, we have tried to keep in mind the students who come across X-ray diffraction crystallography for powder samples at the first time. The primary objective is to offer a textbook to students with almost no basic knowledge of X-rays and a guidebook for young scientists and engineers engaged in full-scale materials development with emphasis on practical problem solving. For the convenience of readers, some essential points with basic equations

are summarized in each chapter, together with some relevant physical constants and atomic scattering factors of elements listed in appendices.

Since practice perfects the acquisition of skills in X-ray diffraction crystallography, 100 supplementary problems are also added with simple solutions. We hope that the students will try to solve these supplementary problems by themselves to deepen their understanding and competence of X-ray crystallography without serious difficulty. Since the field of X-ray structural analysis of materials is quite wide, not all possible applications are covered. The subject matter in this book is restricted to fundamental knowledge of X-ray diffraction crystallography for powder samples only. The readers can refer to specialized books for other applications.

The production of high-quality multi-layered thin films with sufficient reliability is an essential requirement for device fabrication in micro-electronics. An iron-containing layered oxy-pnictide  $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$  has received much attention because it exhibits superconductivity below 43 K as reported recently by Dr. Hideo Hosono in Japan. The interesting properties of such new synthetic functional materials are linked to their periodic and interfacial structures at a microscopic level, although the origin of such peculiar features has not been fully understood yet. Nevertheless, our understanding of most of the important properties of new functional materials relies heavily upon their atomic scale structure. The beneficial utilization of all materials should be pursued very actively to contribute to the most important technological and social developments of the twenty-first century harmonized with nature. Driven by environmental concerns, the interest in the recovery or recycling of valuable metallic elements from wastes such as discarded electronic devices will grow significantly over the next decade. The atomic scale structure of various materials in a variety of states is essential from both the basic science and the applied engineering points of view. Our goal is to take the most efficient approach for describing the link between the atomic scale structure and properties of any substance of interest.

The content of this book has been developed through lectures given to undergraduate or junior-level graduate students in their first half (Master's program) of the doctoral course of the graduate school of engineering at both Tohoku and Kyoto universities. If this book is used as a reference to supplement lectures in the field of structural analysis of materials or as a guide for a researcher or engineer engaged in structural analysis to confirm his or her degree of understanding and to compensate for deficiency in self-instruction, it is an exceptional joy for us.

Many people have helped both directly or indirectly in preparing this book. The authors are deeply indebted to Professors Masahiro Kitada for his valuable advice on the original manuscript. Many thanks are due to Professor K.T. Jacob (Indian Institute of Science, Bangalore), Professor N.J. Themelis (Columbia University), Professor Osamu Terasaki (Stockholm University) and Dr. Daniel Grüner and Dr. Karin Söderberg (Stockholm University) and Dr. Sam Stevens (University of Manchester) who read the manuscript and made many helpful suggestions.

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Note: A solution manual for 100 supplementary problems is available to instructors who have adopted this book for regular classroom use or tutorial seminar use. To obtain a copy of the solution manual, a request may be delivered on your departmental letterhead to the publisher (or authors), specifying the purpose of use as an organization (not personal).

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Introduction, Examples and Solved Problems

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