# Preface

**Aims and Scope of the Book** Materials are important to mankind because of their properties such as electrical conductivity, strength, magnetization, toughness, and numerous others. All these properties originate with the internal structures of materials. Structural features of materials include their types of atoms, the local configurations of the atoms, and arrangements of these configurations into microstructures. The characterization of structures on all these spatial scales is often best performed by transmission electron microscopy and diffractometry, which are growing in importance to materials engineering and technology. Likewise, the internal structures of materials are the foundation for the science of materials. Much of materials science has been built on results from transmission electron microscopy and diffractometry of materials.

This textbook was written for advanced undergraduate students and beginning graduate students with backgrounds in physical science. Its goal is to acquaint them, as quickly as possible, with the central concepts and some details of transmission electron microscopy (TEM) and x-ray diffractometry (XRD) that are important for the characterization of materials. The topics in this book are developed to a level appropriate for most modern materials characterization research using TEM and XRD. The content of this book has also been chosen to provide a fundamental background for transitions to more specialized techniques of research, or to related techniques such as neutron diffractometry. The book includes many practical details and examples, but it does not cover some topics important for laboratory work such as specimen preparation methods for TEM.

Beneath the details of principle and practice lies a larger goal of unifying the concepts common to both TEM and XRD. Coherence and wave interference are conceptually similar for both x-ray waves and electron wavefunctions. In probing the structure of materials, periodic waves and wavefunctions share concepts of the reciprocal lattice, crystallography, and effects of disorder. X-ray generation by inelastic electron scattering is another theme common to both TEM and XRD. Besides efficiency in teaching, a further benefit of an integrated treatment is breadth – it builds strength to apply Fourier transforms and convolutions to examples from both TEM and XRD. The book follows a trend at research universities away from courses focused on one experimental technique, towards more general courses on materials characterization.

The methods of TEM and XRD are based on how wave radiations interact with individual atoms and with arrays of atoms. A textbook must elucidate these interactions, even if they have been known for many years. Figure 1.12, for example, presents Moseley's data from 1914 because this figure is a handy reference today. On the other hand, high-resolution transmission electron microscopy (HRTEM), and the availability of synchrotron and neutron sources for materials research, are important developments that enable wave-matter interactions to probe the structures of materials in new ways. A textbook must integrate both these classical and modern phenomena. The content is a confluence of the old and the new, from both materials science and physics.

**Content** The first two chapters provide a general description of diffraction, imaging, and instrumentation for XRD and TEM. This is followed in Chapters 3 and 4 by electron and x-ray interactions with atoms. The atomic form factor for elastic scattering, and especially the cross sections for inelastic electron scattering, are covered with more depth than needed to understand Chapters 5–7, which emphasize diffraction, crystallography, and diffraction contrast. In a course oriented towards diffraction and microscopy, it is possible to take an easier path through only Sects. 3.1, 3.2.1, 3.2.3, 3.3.2, and the subsection in 3.3.3 on Thomas–Fermi and Rutherford models. Similarly, much of Sect. 4.4 on core excitations could be deferred for advanced study.

The core of the book develops kinematical diffraction theory in the Laue formulation to treat diffraction phenomena from crystalline materials with increasing amounts of disorder. The phase-amplitude diagram is used heavily in Chapter 7 for the analysis of diffraction contrast in TEM images of defects. After a treatment of diffraction lineshapes in Chapter 8, the Patterson function is used in Chapter 9 to treat short-range order phenomena, thermal diffuse scattering, and amorphous materials. High-resolution TEM imaging and image simulation follow in Chapter 10, and the essentials of the dynamical theory of electron diffraction are presented in Chapter 11.

With a discussion of the effective extinction length and the effective deviation parameter from dynamical diffraction, we extend the kinematical theory as far as it can go for electron diffraction. We believe this approach is the right one for a textbook because kinematical theory provides a clean consistency between diffraction and the structure of materials. The phase-amplitude diagram, for example, is a practical device for interpreting defect contrast, and is a handy conceptual tool even when working in the laboratory or sketching on table napkins. Additionally, expertise with Fourier transforms is valuable outside the fields of diffraction and microscopy.

Although Fourier transforms are mentioned in Chapter 2 and used in Chapter 3, their manipulations become more serious in Chapters 4, 5 and 7. Chapter 8 presents convolutions, and the Patterson function is presented in Chapter 9. The student is advised to become comfortable with Fourier transforms at this level before reading Chapters 10 and 11 on HRTEM and dynamical theory. The mathematical level is necessarily higher for HRTEM and dynamical theory, which are grounded in the quantum mechanics of the electron wavefunction.

**Teaching** This textbook evolved from a set of notes for the one-quarter course MS/APh 122 *Diffraction Theory and Applications*, offered to graduate students and advanced undergraduates at the California Institute of Technology, and notes for the one-semester graduate courses MSE 703 *Transmission Electron Microscopy* and MSE 706 *Advanced TEM*, at the University of Virginia. Most of the students in these courses were specializing in materials science or applied physics, and had some background in elementary crystallography and wave mechanics. For a one-semester course (14 weeks) on introductory TEM, one of the authors covers the sections: 1.1, 2.1-2.8, 3.1, 3.3, 4.1-4.3, 4.6, 5.1-5.6, 6.1-6.3, 7.1-7.14. In a course for graduate students with a strong physics background, the other author has covered the full book in 10 weeks by deleting about half of the "specialized" topics.

The choice of topics, depth, and speed of coverage are matters for the taste and discretion of the instructor, of course. To help with the selection of course content, the authors have indicated with an asterisk, "*," those sections of a more specialized nature. The double dagger, "‡," warns of sections containing a higher level of mathematics, physics, or crystallography. Each chapter includes several, sometimes many, problems to illustrate principles. The text for some of these problems includes explanations of phenomena that seemed too specialized for inclusion in the text itself. Hints are given for some of the problems, and worked solutions are available to course instructors. Exercises for an introductory laboratory course are presented in an Appendix.

When choosing the level of presentation for a concept, the authors faced the conflict of balancing rigor and thoroughness against clarity and conciseness. Our general guideline was to avoid direct citations of rules, but instead to provide explanations of the underlying physical concepts. The mathematical derivations are usually presented in steps of equal height, and we try to highlight the central tricks even if this means reviewing elementary concepts. The authors are indebted to our former students for identifying explanations and calculations that needed clarification or correction.

**Acknowledgements** We are grateful for the advice and comments of Drs. C. C. Ahn, D. H. Pearson, H. Frase, U. Kriplani, N. R. Good, C. E. Krill, Profs. L. Anthony, L. Nagel, M. Sarikaya, and the help of P. S. Albertson with manuscript preparation. N. R. Good and J. Graetz performed much of the mathematical typesetting, and we are indebted to them for their careful work. Prof. P. Rez suggested an approach to treat dynamical diffraction in a unified manner. Both authors acknowledge the National Science Foundation for financial support over the years.

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November, 2000