edited by

Oliver H. Seeck
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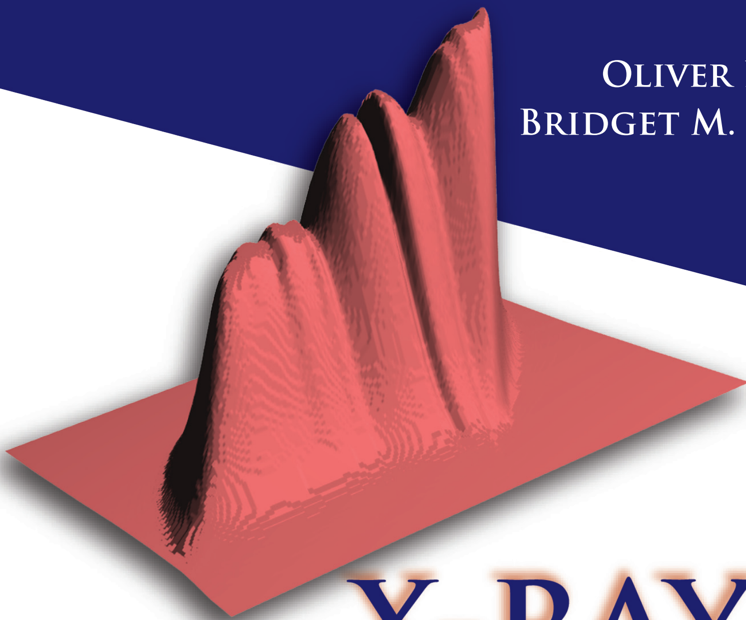
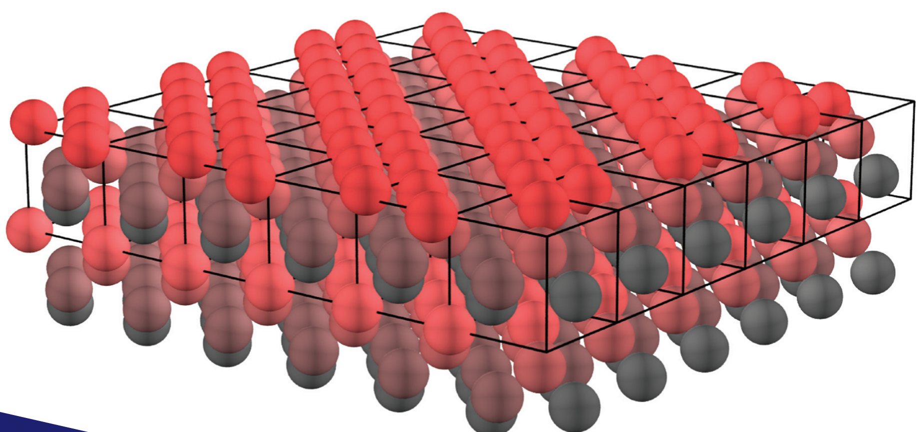


X-RAY DIFFRACTION

Modern Experimental Techniques



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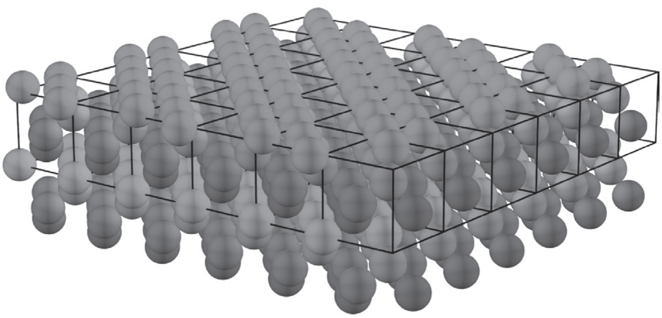

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Contents

Preface

The development of human culture accompanies the progressive understanding of nature. In the last few centuries, the progress was tremendous, especially upon realization that nature is based on complex interplay between interactions on microscopic and macroscopic scale. Regarding the properties of matter, microscopic interactions, in particular between the atoms, are of eminent importance and they basically determine all characteristics. Even fully macroscopic properties such as melting point, viscosity, and stiffness are based on interatomic and intermolecular interaction parameters. To accomplish detailed understanding of the microscopic aspects of nature, science fields such as atomic physics, materials science, chemistry, and theoretical biology have been established. During the past decade, the focus has been additionally put on engineering and technology applications, resulting in the so-called micro- and nanotechnology. In the 21st century, the miniaturization and use of nanomaterials is omnipresent, e.g., in computer and sensor technology and in optics, medicine, and cosmetics; the future potentials are huge.

For further advancements in micro- and nanotechnology, profound knowledge of the interatomic and intermolecular interaction parameters is essential. On the one hand, this is challenging for theoretical science groups that develop mathematical tools to understand nature. On the other hand, experimental tools have to be designed and utilized to actually probe the interactions on the atomic scale. Therefore, scientific instruments with methods based on electrons, ions, or photons have been designed. Some of them are available as (more or less) inexpensive laboratory equipment. However, for high-end applications, they can be very costly and complex with a need of well-trained personnel for operation.

Tremendous progress has been achieved in the development of tools based on X-radiation. During the past 50 years, the evolution went from laboratory sources, so-called X-ray tubes, which are still available today, to parasitic use of synchrotron radiation from particle physics experiments, dedicated storage rings for X-radiation, and finally to X-ray lasers. The latter two are large-scale facilities with construction costs of several hundred million US dollars up to USD 1 billion and significant manpower with hundreds of FTEs to run the experiments. All over the world, approximately 20 modern sources are available, of which four deliver high-energy photons and two X-ray lasers. Synchrotron radiation sources offer extraordinary high X-ray beam quality for high-precision measurements on the atomic or molecular scale with accessible time scales from seconds down to femtoseconds (in the case of X-ray lasers). At each of the sources, a large number of experimental stations have been accommodated, which are specialized on certain X-ray methods, such as micro-diffraction, small-angle scattering, X-ray photo emission, fluorescence spectroscopy, tomography, and many more.

Modern synchrotron radiation sources are available for the general scientific and industrial community. Users are mostly from fields in physics, chemistry, geoscience, materials science, biology, archeology, and related fields. Usually, beam time is distributed on a proposal-based system with external referees. For this, an applicant has to define the science case and to choose an experimental station that fits his purpose best. At this point, a potential user should be able to evaluate the capabilities of the experimental stations at the synchrotron radiation sources and to identify the X-ray methods that he wants to apply. Aside from the experimental station, the X-ray photon flux and energy, the beam size and the divergence, the coherence and timing are properties of eminent importance.

In this book, the most important X-ray scattering and diffraction methods are introduced along with some aspects about the production of X-radiation at synchrotrons. In the first two chapters, the basics of X-ray diffraction and scattering methods and an overview of the characteristics of synchrotron radiation are presented. Also, the X-ray optics of a synchrotron radiation experiment are explained, which enables the reader to estimate the flux and the other beam parameters at the sample. In the later chapters, experts explain the different scattering and diffraction techniques.

The chapters on micro-diffraction and small-angle scattering give insights into the research of macromolecular samples, crystalline or amorphous. For both methods, focusing of the beam is of eminent importance; therefore, in the micro-diffraction section, focusing techniques are introduced. The following two chapters focus on inelastic scattering and X-ray standing waves, which are widely used to investigate phonon- and electron-density distribution in hard condensed matter. The next two chapters are devoted to magnetism. Two fully different X-ray methods are applicable: Magnetic scattering, which is a diffraction method based on magnetic interaction with the X-rays, and nuclear scattering, which monitors changes in the hyperfine field of the nuclei induced by magnetism in the sample.

The three following chapters deal with special topics: scattering at liquid interfaces, extreme condition science with X-rays, and tomography. The first is demanding as many chemical and biological reactions appear at liquid interfaces. Extreme condition science (high temperature and high pressure) relies on well-established X-rays powder diffraction methods; however, the experimental setup is very complex and the present status is explained in the book. Tomography is also introduced, though it is not a particular scattering or diffraction method. In many cases, such as metallic sintered powders, tomography and scattering methods are complementary.

The last two chapters describe applications of coherent X-rays. The so-called speckle pattern that arises from scattering of coherent beams at disordered samples contains more information than standard scattering data and can be used to do imaging or time-resolved studies. The experimental techniques and the rather complex theory are introduced in these chapters.

This book gives an insight into the up-to-date X-ray scattering methods that are available at modern synchrotron radiation sources. It enables the reader to understand the basic concept behind the methods and therefore to plan an appropriate, synchrotron radiation–based experiment.