Structure Analysis by Small-Angle X-Ray and Neutron Scattering

Intermetallics

Molecular Structure

A concise introduction to modern crystal structure determination, emphasizing both the crystallographic background and the successive practical steps. In the theoretical sections, more importance is attached to a good understanding, than to a rigorous mathematical treatment. The most important measuring techniques, including the use of modern area detectors, and the methods of data analysis are described. The book is divided into two parts: the first part covers the basics of crystallography and diffraction, while the second part focuses on molecular structure determination.

The book is intended for graduate students and researchers in chemistry, physics, and materials science, as well as for practitioners in industry and academia. It provides a comprehensive overview of the current state of the art in crystal structure determination, with a focus on the practical aspects of the process.
Red Online Crystal Structure Analysis Principles And Practice International Union Of Crystallography Monographs On Crystallography

reduction, structure solution and refinement are discussed from a practical point of view. Special emphasis is put on the ability to recognize and avoid possible errors and traps, and to judge the quality of results.

Crystal Symmetries

Elements of X Ray Diffraction Small-angle scattering of X rays and neutrons is a widely used diffraction method for studying the structure of matter. This method of elastic scattering is used in various branches of science and technology, including condensed matter physics, molecular biology and biophysics, polymer science, and metallurgy. Many small-angle scattering studies are of value for pure science and practical applications. It is well known that the most general and informative method for investigating the spatial structure of matter is based on wave-diffraction phenomena. In diffraction experiments a primary beam of radiation influences a studied object, and the scattering pattern is analyzed. In principle, this analysis allows one to obtain information on the structure of a substance with a spatial resolution determined by the wavelength of the radiation. Diffraction methods are used for studying matter on all scales, from elementary particles to macro-objects. The use of X rays, neutrons, and electron beams, with wavelengths of about 1 Å, permits the study of the condensed state of matter, solids and liquids, down to atomic resolution. Determination of the atomic structure of crystals, i.e., the arrangement of atoms in a unit cell, is an important example of this line of investigation.

Crystal Structure Refinement


Perspectives in Crystallography

By choosing an approach that avoids undue emphasis on the mathematics involved, this book gives practical advice on topics such as growing crystals, solving and refining structures, and understanding and using the results.
Read Online Crystal Structure Analysis Principles And Practice International Union Of Crystallography Monographs On Crystallography

The book is designed to be used as a text for teaching students about the capabilities and limitations of the powder diffraction method. It is still meant to be used as a text for teaching students about the capabilities and limitations of the powder diffraction method. We also hope that it goes beyond a simple text, and therefore, is useful as a reference to practitioners of the technique. The original book had seven long chapters that may have made its use as a text inconvenient. So the second edition is broken down into 25 shorter chapters. The first fifteen are concerned with the fundamentals of powder diffraction, which makes it much more logical, considering a typical 16-week long semester. The last ten chapters are concerned with practical examples of structure solution and refinement, which were preserved from the first edition and expanded by another example: solving the crystal structure of Tylenol.

Structural Science of Crystalline Polymers X-ray crystallography supplies chemists, mineralogists, material scientists, molecular biologists with precise and direct information on crystal and molecular structures of substances and intermolecular interactions. This text provides an up-to-date overview of crystallographic instrumentation and methods of diffraction measurements used for crystal and molecular structure determination. The book provides a unique description of both principles and specific instruments, and methods for data collection, adjustment of instruments, and primary data processing and error correction.

Crystals, X-rays and Proteins The fields of structural chemistry and biochemistry have blossomed in the last seventy years since X-ray diffraction was discovered in 1912. Dorothy Hodgkin, who obtained a Nobel Prize in 1965 for her X-ray diffraction work wrote 'a great advantage of X-ray analysis as a method of chemical structure analysis is its power to show some totally unexpected and surprising structure with, at the same time, complete certainty.' The results of all X-ray diffraction studies are used by chemists and biochemists but these scientists need to be able to appreciate the significance and extent to which these results may be used. A number of books written for practicing crystallographers cover the theory and applications of X-ray diffraction, but few are of real practical use to non-specialists. In 'Crystal Structure Analysis for Biologists and Chemists', the general principles of crystal structure are presented in a highly readable way. The book of Glusker, who is internationally renowned, provides good coverage of theory, including data and understanding their significance.

Chemistry and Applications of Benzimidazole and its Derivatives This classic text is devoted to describing crystal structures, especially periodic structures, and their symmetries. Updated material prepared by the author enhances presentation, which can serve as text or reference. 1996 edition.

Crystal Structure Determination X-ray crystallography is the main method used to determine the structure of biological molecules. X-ray crystallography is explained without maths and reading this text allows biologists to assess the quality and accuracy of biological structures.

Crystal Structure Analysis for Chemists and Biologists Finding new strategies for synthesizing benzimidazole derivatives and functionalizing the benzimidazole core has proved to be important due to the compound's various applications in medicine, chemistry, and other areas. The multitude of benzimidazole derivatives marketed as drugs has led to intensive research in the field for the discovery of new biologically active structures. The general applications of benzimidazole derivatives in materials chemistry, electronics, technology, dyes, pigments, and agriculture open up new research horizons. This book guides the rational design of benzimidazole derivatives synthesis with certain applications. Chapters cover such topics as therapeutic use of benzimidazole in conditions like diabetes, viruses, and parasitic diseases; X-ray crystal structure of selected benzimidazole derivatives; benzimidazole compounds for cancer therapy; and others.
Crystalline materials are widely used in everyday life and various industrial applications. The study of their structure, known as crystallography, is crucial for understanding their properties and performance. This field involves the use of x-rays, neutrons, and other radiation sources to analyze the internal arrangements of atoms in a crystal.

Early workers in the field, such as W.L. Bragg, made significant contributions to the development of x-ray crystallography. In 1912, they published a paper that introduced the concept of Bragg's Law, which relates the wavelength of x-rays to the spacing of crystal planes. This law has since become the cornerstone of x-ray crystallography.

In the 1930s, M.oux developed the Patterson method, which involves the analysis of the convolution of the electron density. This method was later refined and expanded by other researchers, leading to the development of more advanced techniques such as direct methods and molecular replacement.

During World War II, crystallography was overshadowed by research focused on practical applications, but it saw a resurgence in the post-war period. The development of faster computers and the introduction of new technologies, such as synchrotrons, have significantly improved the accuracy and speed of crystallographic analysis.

Today, crystallography is an essential tool in scientific research, with applications ranging from material science and chemistry to biology and medicine. The ability to determine the atomic structure of materials at high resolution is critical for understanding their physical properties and predicting their behavior under various conditions.

The Handbook on Crystallography and Crystal Defects offers a comprehensive overview of the field, covering both theoretical and practical aspects. It is an invaluable resource for students, researchers, and professionals interested in crystallography and its applications.
The advances in and applications of x-ray and neutron crystallography form the essence of this new edition of this classic textbook, while maintaining the overall plan of the book that has been well received in the academic community since the first edition in 1977. X-ray crystallography is a universal tool for studying molecular structure, and the complementary nature of neutron diffraction crystallography permits the location of atomic species in crystals which are not easily revealed by X-ray techniques alone, such as hydrogen atoms or other light atoms in the presence of heavier atoms. Thus, a chapter discussing the practice of neutron diffraction techniques, with examples, broadens the scope of the text in a highly desirable way. As with previous editions, the book contains problems to illustrate the work of each chapter, and detailed solutions are provided. Mathematical procedures related to the material of the main body of the book are not discussed in detail, but are quoted where needed with references to standard mathematical texts. To address the computational aspect of crystallography, the suite of computer programs from the fourth edition has been revised and expanded. The programs enable the reader to participate fully in many of the aspects of x-ray crystallography discussed in the book. In particular, the program system XRAY* is interactive, and enables the reader to follow through, at the monitor screen, the computational techniques involved in single-crystal structure determination, albeit in two dimensions, with the data sets provided. Exercises for students can be found in the book, and solutions are available to instructors.
Read Online Crystal Structure Analysis Principles And Practice International Union Of Crystallography Monographs On Crystallography

Crystal Structure Analysis Principles And Practice International Union Of Crystallography Monographs On Crystallography

Crystal Structure Analysis Crystals and Crystal Structures is an introductory text for students and others who need to understand the subject without necessarily becoming crystallographers. Using the book will enable students to read scientific papers and articles describing a crystal structure or use crystallographic databases with confidence and understanding. Reflecting the interdisciplinary nature of the subject the book includes a variety of applications as diverse as the relationship between physical properties and symmetry, and molecular and protein crystallography. As well as covering the basics the book contains an introduction to areas of crystallography, such as modulated structures and quasicrystals, and protein crystallography, which are the subject of important and active research. A non-mathematical introduction to the key elements of the subject Contains numerous applications across a variety of disciplines Includes a range of problems and exercises Clear, direct writing style “the book contains a wealth of information and it fulfils its purpose of providing an interesting and broad introduction to the terpenes.” CHEMISTRY WORLD, February 2007

Recent Advances in Crystallography This concise text describes the basic principles of crystal structure determination by X-ray diffraction and the application of these principles in practice. The technique is presented step-by-step and illustrated with a wide range of case studies, including the use of the most up-to-date equipment. Crystal Structure Determination explains how X-ray crystallography fits in with modern chemistry, why it is important, and what it can do, with the aim of enabling the reader to understand and assess structural results in books and research journals. There is additional coverage of related topics such as neutron diffraction and the application of computer databases. Mathematical treatment is kept at a relatively low level and is complemented by extensive illustrations and worked examples. This clear introduction to the topic will be an essential text for chemistry undergraduates. Other related science undergraduates (biochemists, environmental scientists, etc.) and postgraduate chemists will also find this book useful.

Outline of Crystallography for Biologists

The Theory of Crystal Structure Analysis This book provides a clear introduction to topics which are essential to students in a wide range of scientific disciplines but which are otherwise only covered in specialised and mathematically detailed texts. It shows how crystal structures may be built up from simple ideas of atomic packing and co-ordination, it develops the concepts of crystal symmetry, point and space groups by way of two dimensional examples of patterns and tilings, it explains the concept of the reciprocal lattice in simple terms and shows its importance in an understanding of light, X-ray and electron diffraction. Practical examples of the applications of these techniques are described and also the importance of diffraction in the performance of optical instruments. The book is also of value to the general reader since it shows, by biographical and historical references, how the subject has developed and thereby indicates some of the excitement of scientific discovery.

Crystal Structure Analysis Crystallography is one of the most multidisciplinary sciences, with roots in fields as varied as mathematics, physics, chemistry, biology, materials science, computation and earth and planetary science. The structural knowledge gained from crystallography has been instrumental in acquiring new levels of understanding in numerous scientific areas. Perspectives in Crystallography provides an overview of the current state of the field, reviews its historical origins and explains how crystallography contributes to the sustainability of life. This book resonates with the recent United Nations and UNESCO International Year of Crystallography, a celebration of its achievements and importance, undertaken with the International Union of Crystallography. The author of this book is the editor in chief of Crystallography Reviews, where some of the contents have been previously published. Here, subjects of interest to specialists and non-specialists have been brought together in a single source. The book opens with a description of the ways to explain crystallography to diverse general audiences. It also addresses various topics in crystallography, including: The evolution and importance of synchrotron radiation to crystallography The structural chemistry and biology of colouration in marine crustacea Predicting protonation states of proteins versus crystallographic experimentation The book then offers a projection of crystal structure analysis in the next 100 years and concludes by emphasizing the societal impacts of crystallography that allow for sustainability of life. Perspectives in Crystallography offers a threefold look into the past, present and long-term development and relevance of crystal structure analysis. It is concerned not only with the state of the field, but with its role in the perpetuation of life on earth. As such, it is a reference of vital interest to a broad range of analytical and practical sciences.
The advent of X-ray diffraction in the early twentieth century transformed crystallography from an area of scientific inquiry largely limited to physics, mineralogy, and mathematics, to a highly interdisciplinary field which now includes nearly all life and physical sciences as well as materials science and engineering. This book is a collection of works showcasing some of the most recent developments in the field of crystallography.

The Basics of Crystallography and Diffraction

Crystallography may be described as the science of the structure of materials, using this word in its widest sense, and its ramifications are apparent over a broad front of current scientific endeavor. It is not surprising, therefore, to find that most universities offer some aspects of crystallography in their undergraduate courses in the physical sciences. It is the principal aim of this book to present an introduction to structure determination by X-ray crystallography that is appropriate mainly to both final-year undergraduate studies in crystallography, chemistry, and chemical physics, and introductory postgraduate work in this area of crystallography. We believe that the book will be of interest in other disciplines, such as physics, metallurgy, biochemistry, and geology, where crystallography has an important part to play. In the space of one book, it is not possible either to cover all aspects of crystallography or to treat all the subject matter completely rigorously. In particular, certain mathematical results are assumed in order that their applications may be discussed. At the end of each chapter, a short bibliography is given, which may be used to extend the scope of the treatment given here. In addition, reference is made in the text to specific sources of information. We have chosen not to discuss experimental methods extensively, as we consider that this aspect of crystallography is best learned through practical experience, but an attempt has been made to simulate the interpretive side of experimental crystallography in both examples and exercises.

Crystal Structure Analysis

The concepts of crystallography are introduced here in such a way that the physical properties of crystals, including their mechanical behaviour, can be better understood and quantified. A unique approach to the treatment of crystals and their defects is taken in that the often separate disciplines of crystallography, tensor analysis, elasticity and dislocation theory are combined in such a way as to equip materials scientists with knowledge of all the basic principles required to interpret data from their experiments. This is a revised and updated version of the widely acclaimed book by Kelly and Groves that was first published nearly thirty years ago. The material remains timely and relevant and the first edition still holds an unrivalled position at the core of the teaching of crystallography and crystal defects today. Undergraduate readers will acquire a rigorous grounding, from first principles, in the crystal classes and the concept of a lattice and its defects and their descriptions using vectors. Researchers will find here all the theorems of crystal structure upon which to base their work and the equations necessary for calculating interplanar spacings, transformation of indices and manipulations involving the stereographic projection and transformations of tensors and matrices.

NMR Crystallography

The book describes phasing techniques in modern crystallography. The main text is dedicated to their simple description, and further mathematical details are contained in the appendices. Practical aspects are described for each specific method, making it a useful tool for the daily work of practising crystallographers.


The purpose of this book is to explain why molecular structure can be determined by single-crystal diffraction of X-rays. It is not an account of the practical procedural details, but rather an account of the underlying physical principles, and the kinds of experiments and methods of handling the experimental data that are used.

Crystallography

The fascinating world of intermetallics is largely unexplored. There are many exciting physical properties and important technological applications of intermetallics, from magnetism to superconductivity. The main focus of this book is on the statistics, topology and geometry of crystal structures and structure types of intermetallic phases. The underlying physics, in particular chemical bonding, is discussed whenever it helps understand the stability of structures and the origin of their physical properties. The authors’ approach, based on the statistical analysis of more than twenty thousand intermetallic compounds in the database Pearson’s Crystal Data, uncovers important structural relationships and illustrates the relative simplicity of most of the general structural building principles. It
The text aims to be readable and beneficial in one way or another to everyone interested in intermetallic phases, from graduate students to experts in solid state chemistry and physics, and materials science. For that purpose it avoids the use of enigmatic abstract terminology for the classification of structures. Instead, it focuses on the statistical analysis of crystal structures and structure types in order to draw together a larger overview of intermetallics, and indicate the gaps in it - areas still to be explored, and potential sources of worthwhile research. The text should be read as a reference guide to the incredibly rich world of intermetallic phases.

Crystals and Crystallinity in Polymers This textbook gives a concise introduction to modern crystal structure determination, emphasising both its theoretical background and the way it is actually carried out. The theoretical sections are supported by many illustrations, and lay emphasis on a good understanding rather than rigorous mathematics. The most important data collection techniques, and the methods of data reduction, structure solution and refinement are discussed from a practical point of view. Many tips and insights help readers to recognise and avoid possible errors and traps, and to judge the quality of results. The second edition has been considerably updated, especially the chapter on experimental methods, which is now mainly concerned with modern data collection using area-detectors.

Powder Diffraction This book is a printed edition of the Special Issue "Rietveld Refinement in the Characterization of Crystalline Materials" that was published in Crystals.