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Dr. Peter H. Ravn

Dr. Peter H. Ravn

Mathematical Techniques In Crystallography And Materials Science

H.-J. Bunge



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Mathematical Techniques in Crystallography and Materials Science Edward Prince, 2004-03-23 Mathematical techniques in Crystallography and Materials Science brings together common and less familiar mathematical procedures used in studies of the structures and physical properties of solids This practical guide and reference serves as a unified source book for students and professionals and it provides a solid basis for further studies in more specialized literature

Mathematical Techniques in Crystallography and Material Science Edward Prince, 2012-02 Crystallographers have to apply many mathematical methods in their daily work If ever they have a problem this book will help to solve it The newcomer starting work will learn how to apply these tools the practicing crystallographer will find all the data and background material he wants to look up In the decade since the first edition was published new things have happened that required revision beyond correction of errors Two chapters have been added a section on the projection matrix and another on fast Fourier Transform The author collected the information during his professional career The success of the first edition indicates that many other practicing crystallographers just need exactly that information Mathematical Techniques in Crystallography and Materials Science E. Prince, 1982-03-08 **Texture Analysis in Materials Science** H.-J.

Bunge, 2013-09-03 Texture Analysis in Materials Science Mathematical Methods focuses on the methodologies processes techniques and mathematical aids in the orientation distribution of crystallites The manuscript first offers information on the orientation of individual crystallites and orientation distributions Topics include properties and representations of rotations orientation distance and ambiguity of rotation as a consequence of crystal and specimen symmetry The book also takes a look at expansion of orientation distribution functions in series of generalized spherical harmonics fiber textures and methods not based on the series expansion The publication reviews special distribution functions texture transformation and system of programs for the texture analysis of sheets of cubic materials The text also ponders on the estimation of errors texture analysis and physical properties of polycrystalline materials Topics include comparison of experimental and recalculated pole figures indetermination error for incomplete pole figures and determination of the texture coefficients from anisotropic polycrystal properties The manuscript is a dependable reference for readers interested in the use of mathematical aids in the orientation distribution of crystallites Current Methods and Optimization Algorithms for the Refinement of X-Ray Crystal Structures J Uria, 1999-08-19 Fundamentals of Powder Diffraction and Structural Characterization of Materials Peter Y.

Zavalij, Vitalij K. Pecharsky, 2025-09-26 This expanded updated third edition features many new color illustrations timely practical examples and experimental and computational tools introduced in the past ten years while retaining its excellent introduction to structural characterization and crystallography The book is written for those interested in a fundamental conceptual understanding powder diffraction and structural characterization of materials as well as in practical skills in examining phase composition and structure of materials using modern experimental powder diffraction tools Special

attention is given to proper collection of powder diffraction data using laboratory x ray synchrotron and neutron radiation Exemplary data sets serve as a springboard for readers to develop knowledge about modern approaches algorithms and software as well as to gain proficiency in extracting precise structural information about crystalline materials from powder diffraction data The book requires no specialized knowledge so it is useful to beginners Suitable for upper level undergraduate and graduate students as well as practitioners in the research labs and the field the authors in depth treatment helps readers from various disciplines including crystallography materials science solid state chemistry and physics geology and mineralogy become experts on this subject

Fundamentals of Powder Diffraction and Structural Characterization of Materials, Second Edition Vitalij Pecharsky, Peter Zavalij, 2008-11-24 A little over five years have passed since the first edition of this book appeared in print Seems like an instant but also eternity especially considering numerous developments in the hardware and software that have made it from the laboratory test beds into the real world of powder diffraction This prompted a revision which had to be beyond cosmetic limits The book was and remains focused on standard laboratory powder diffractometry 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 convenient 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

International Tables for Crystallography, Volume C E. Prince, 2004-01-31 International Tables for Crystallography are no longer available for purchase from Springer For further information please contact Wiley Inc follow the link on the right hand side of this page The purpose of Volume C is to provide the mathematical physical and chemical information needed for experimental studies in structural crystallography The volume covers all aspects of experimental techniques using all three principal radiation types from the selection and mounting of crystals and production of radiation through data collection and analysis to interpretation of results As such it is an essential source of information for all workers using crystallographic techniques in physics chemistry metallurgy earth sciences and molecular biology

Foundations of Crystallography with Computer Applications Maureen M. Julian, Carla Slebodnick, Francis T. Julian, 2024-11-29 The third edition of Foundations of Crystallography with Computer Applications is a textbook for undergraduate and graduate students studying the solid state in chemistry physics materials science geological sciences and engineering It takes a straightforward logical approach to explaining how atoms are arranged in crystals and how crystal systems are related to each other New to this edition is the inclusion of interactive Starter Programs in Python which allow the students to focus on concepts and not treat crystallographic programs as black

boxes Since many students have trouble visualizing three dimensional constructions this book begins with detailed discussions in two dimensions leading up to the three dimensional understanding The first seven chapters introduce the fundamental principles Chapter 8 suggests student projects and the final seven chapters give detailed examples of the seven crystal systems Key features Uses Python the leading open source scientific language with libraries including NumPy for matrix manipulations Matplotlib for graphics and Mplot3d for interactive 3 D modeling Provides a gentle introduction to Python with Jupyter Notebooks which combine interactive code and formatted documentation Color codes both point group and space group diagrams using a new scheme devised by the author to emphasize the change of handedness of the symmetry operations and their consequences Suggests student projects with data that can be found in the free Teaching Subset of the Cambridge Structural Database the American Mineralogist Crystal Structure Database and others This book s thorough but accessible style gives students a strong foundation in the subject Over one thousand students have successfully used this book at Virginia Tech and many more will continue to benefit from this new edition

Crystal Structure Analysis for Chemists and Biologists Jenny P. Glusker, Mitchell Lewis, Miriam Rossi, 1996-12-17 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 buiochemists 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

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