

# The Rietveld Method

The **Rietveld Method** consists of refining a crystal (and/or magnetic) structure by minimising the weighted squared difference between the observed and the calculated pattern against the parameter vector:  $\mathbf{P}$

$$\chi^2 = \sum_{i=1}^n w_i (y_i - y_{ci}(\mathbf{P}))^2$$

$$w_i = \frac{1}{\sigma_i^2}$$

$\sigma_i^2$ : is the variance of the "observation"  $y_i$

# Rietveld Method

**Karen Scrivener, Ruben  
Snellings, Barbara Lothenbach**



## **Rietveld Method:**

**The Rietveld Method** Robert Alan Young, 1993 The Rietveld method is a powerful and relatively new method for extracting detailed crystal structural information from X ray and neutron powder diffraction data Since such structural details dictate much of the physical and chemical attributes of materials knowledge of them is crucial to our understanding of those properties and our ability to manipulate them Since most materials of technological interest are not available as single crystals but often are available only in polycrystalline or powder form the Rietveld method has become very important and is now widely used in all branches of science that deal with materials at the atomic level This book a collaboration by many authorities in the field is intended primarily to have tutorial and advisory value for those who already have some experience with this important method but an introductory chapter enables the book to be used as a first text for researchers starting in this area of science The audience is thus comprised of all scientists using the method graduate students who may be starting research in this area powder diffraction specialists crystallographers physicists chemists and materials scientists

**Fundamentals of Powder Diffraction and Structural Characterization of Materials** Vitalij Pecharsky, Peter Zavalij, 2003-05-31 Requires no prior knowledge of the subject but is comprehensive and detailed making it useful for both the novice and experienced user of the powder diffraction method Useful for any scientific or engineering background where precise structural information is required Comprehensively describes the state of the art in structure determination from powder diffraction data both theoretically and practically using multiple examples of varying complexity Pays particular attention to the utilization of Internet resources especially the well tested and freely available computer codes designed for processing of powder diffraction data

**Fundamentals of Powder Diffraction and Structural Characterization of Materials, Second Edition** Vitalij Pecharsky, Peter Zavalij, 2008-11-24 A little over ve years have passed since the rst 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 rst fteen are concerned with the fundamentals of powder diffraction which makes it much more logical considering a typical 16 week long semester The last ten ch ters are concerned with practical examples of structure solution and re nement which were preserved from the rst edition and expanded by another example R solving the crystal structure of Tylenol

*Rietveld Made Easy* John Charles Taylor, Ihor Hinczak, 2003 The Rietveld Method is a device developed by Hugo Rietveld in order to determine and caractarize crystalline materials by

means of powder diffraction Part one of this book concerns Non Rietveld XRD analysis using integrated intensities Part two concerns Rietveld a simple extension to the XRD profile from Non Rietveld **Powder Diffraction** Georg Will,2006-01-26

Crystal structure analysis from powder diffraction data has attracted considerable and ever growing interest in the last decades X ray powder diffraction is best known for phase analysis Hanawalt files dating back to the 30s In the late 60s the inherent potential of powder diffraction for crystallographic problems was realized and scientists developed methods for using powder diffraction data at first only for the refinement of crystal structures With the development of ever growing computer power profile fitting and pattern decomposition allowed to extract individual intensities from overlapping diffraction peaks opening the way to many other applications especially to ab initio structure determination Powder diffraction today is used in X ray and neutron diffraction where it is a powerful method in neutron diffraction for the determination of magnetic structures In the last decade the interest has dramatically improved There is hardly any field of crystallography where the Rietveld or full pattern method has not been tried with quantitative phase analysis the most important recent application **Rietveld Refinement** Robert E. Dinnebier,Andreas Leineweber,John S.O.

Evans,2018-12-17 Almost 50 years have passed since the famous papers of Hugo Rietveld from the late sixties where he describes a method for the refinement of crystal structures from neutron powder diffraction data Soon after the potential of the method for laboratory X ray powder diffraction was discovered Although the method is now widely accepted there are still many pitfalls in the theoretical understanding and in practical daily use This book closes the gap with a theoretical introduction for each chapter followed by a practical approach The flexible macro type language of the Topas Rietveld software can be considered as the defacto standard **Powder diffraction : proceedings of the II International School**

**on Powder Diffraction ; January 20 - 23, 2002, IACS, Kolkata, India ; (as part of 125 years of celebration)** S. P. Sen Gupta,2002 *The Rietveld Method* R. A. Young,1993 [A Practical Guide to Microstructural Analysis of Cementitious Materials](#) Karen Scrivener,Ruben Snellings,Barbara Lothenbach,2018-10-09 A Practical Guide from Top Level Industry Scientists As advanced teaching and training in the development of cementitious materials increase the need has emerged for an up to date practical guide to the field suitable for graduate students and junior and general practitioners Get the Best Use of Different Techniques and Interpretations of the Results This edited volume provides the cement science community with a state of the art overview of analytical techniques used in cement chemistry to study the hydration and microstructure of cements Each chapter focuses on a specific technique not only describing the basic principles behind the technique but also providing essential practical details on its application to the study of cement hydration Each chapter sets out present best practice and draws attention to the limitations and potential experimental pitfalls of the technique Databases that supply examples and that support the analysis and interpretation of the experimental results strengthen a very valuable ready reference Utilizing the day to day experience of practical experts in the field this book Covers sample preparation issues

Discusses commonly used techniques for identifying and quantifying the phases making up cementitious materials X ray diffraction and thermogravimetric analysis Presents good practice on calorimetry and chemical shrinkage methods for studying cement hydration kinetics Examines two different applications of nuclear magnetic resonance solid state NMR and proton relaxometry Takes a look at electron microscopy the preeminent microstructural characterization technique for cementitious materials Explains how to use and interpret mercury intrusion porosimetry Details techniques for powder characterization of cementitious materials Outlines the practical application of phase diagrams for hydrated cements Avoid common pitfalls by using *A Practical Guide to Microstructural Analysis of Cementitious Materials* A one of a kind reference providing the do's and don'ts of cement chemistry the book presents the latest research and development of characterisation techniques for cementitious materials and serves as an invaluable resource for practicing professionals specializing in cement and concrete materials and other areas of cement and concrete technology

*Diffraction Analysis of the Microstructure of Materials* Eric J. Mittemeijer, Paolo Scardi, 2003-11-26 Overview of diffraction methods applied to the analysis of the microstructure of materials Since crystallite size and the presence of lattice defects have a decisive influence on the properties of many engineering materials information about this microstructure is of vital importance in developing and assessing materials for practical applications The most powerful and usually non destructive evaluation techniques available are X ray and neutron diffraction The book details among other things diffraction line broadening methods for determining crystallite size and atomic scale strain due e.g. to dislocations and methods for the analysis of residual macroscale stress The book assumes only a basic knowledge of solid state physics and supplies readers sufficient information to apply the methods themselves

Powder Diffraction R E Dinnebier, S J L Billinge, 2015-11-09 Powder diffraction is a widely used scientific technique in the characterization of materials with broad application in materials science chemistry physics geology pharmacology and archaeology *Powder Diffraction Theory and Practice* provides an advanced introductory text about modern methods and applications of powder diffraction in research and industry The authors begin with a brief overview of the basic theory of diffraction from crystals and powders Data collection strategies are described including x ray neutron and electron diffraction setups using modern day apparatus including synchrotron sources Data corrections essential for quantitative analysis are covered before the authors conclude with a discussion of the analysis methods themselves The information is presented in a way that facilitates understanding the information content of the data as well as best practices for collecting and analyzing data for quantitative analysis This long awaited book condenses the knowledge of renowned experts in the field into a single authoritative overview of the application of powder diffraction in modern materials research The book contains essential theory and introductory material for students and researchers wishing to learn how to apply the frontier methods of powder diffraction

**Fifth Size Strain Conference. Diffraction Analysis of the Microstructure of Materials**, 2015-10-29 *Zeitschrift für Kristallographie Supplement Volume 27* presents the complete Proceedings of all

contributions to the V Size Strain Conference in Garmisch Partenkirchen 2007 Lattice Defects Residual Stresses Texture in Thin Films and at Surfaces Line Broadening Analysis and Line Profile Fitting Diffraction Microstructure Modeling Supplement Series of Zeitschrift für Kristallographie publishes Proceedings and Abstracts of international conferences on the interdisciplinary field of crystallography      **Applied Mineralogy of Cement & Concrete** Maarten A.T.M. Broekmans, Herbert Pöllmann, 2018-12-17 Volume 74 of Reviews in Mineralogy and Geochemistry contains a selection of papers on the applied mineralogy of cement and concrete by far the most popular modern building material by volume with an annual production exceeding 9 billion cubic meters and steadily growing Not even all concrete topics can be covered by a single volume but an interesting assortment was finally obtained The seven chapters deal with mineralogy and chemistry of alumina clinker production and hydration Pöllmann alternative raw clinkering materials to reduce CO<sub>2</sub> emission Justnes assessment of clinker constituents by optical and electron microscopy Stutzman industrial assessment of raw materials cement and concrete using X ray methods in different applications Meier et al in situ investigation of clinker and cement hydration based on quantitative crystallographic phase analysis Aranda et al characterization and properties of supplementary cementitious materials SCMs to improve cement and concrete properties Snellings et al and deleterious alkali aggregate reaction AAR in concrete Broekmans      **Modern Powder Diffraction** David L. Bish, Jeffrey E. Post, 2018-12-17 Volume 20 of Reviews in Mineralogy attempted to 1 provide examples illustrating the state of the art in powder diffraction with emphasis on applications to geological materials 2 describe how to obtain high quality powder diffraction data and 3 show how to extract maximum information from available data In particular the nonambient experiments are examples of some of the new and exciting areas of study using powder diffraction and the interested reader is directed to the rapidly growing number of published papers on these subjects Powder diffraction has evolved to a point where considerable information can be obtained from µg sized samples where detection limits are in the hundreds of ppm range and where useful data can be obtained in milliseconds to microseconds We hope that the information in this volume will increase the reader's access to the considerable amount of information contained in typical diffraction data      Solid Oxide Fuel Cell (SOFC) Materials R. Saravanan, 2018-01-15 Developing materials for SOFC applications is one of the key topics in energy research The book focuses on manganite structured materials such as doped lanthanum chromites and lanthanum manganites which have interesting properties thermal and chemical stability mixed ionic and electrical conductivity electrocatalytic activity magnetocaloric property and colossal magnetoresistance CMR These materials have applications in solid oxide fuel cells high temperature NO<sub>x</sub> sensors hard disk read heads magnetic sensors and magnetoresistive random access memories For the first time the charge density distributions have been studied in these materials as synthesized by high temperature solid state reaction Charge density analysis is helpful in understanding the physical and chemical properties of materials and in developing optimized structures The morphological elemental optical and magnetic properties

of the materials have also been studied Solid Oxide Fuel Cells SOFC Manganite Structured Materials Lanthanum Chromites Lanthanum Manganites Electrocatalytic Activity Magnetocaloric Property Colossal Magnetoresistance High Temperature NO<sub>x</sub> Sensors Hard Disk Read Heads Magnetic Sensors Magnetoresistive Random Access Memories Charge Density Distribution Charge Density and Structural Characterization of Thermoelectric Materials R. Saravanan, 2016-06-01 Thermoelectric materials permit the direct conversion of temperature differences into electric energy and vice versa They are therefore of highest technological interest in applications such as solid state coolers waste heat recovery sensors and detectors and power generators including remote power generation Thermoelectric materials are often called environmentally green and for good reasons Not only can they help generate electrical energy from waste gases as they are generated in such processes as home heating industrial fabrication and automotive motion In cooling applications they eliminate the use of chemical refrigerant gases Moreover as thermoelectric conversion devices have no moving parts they operate silently and have a very long life expectancy The only current drawback of these devices is their poor efficiency Scientists all over the world are therefore studying the structural thermoelectric charge density and magnetic properties of the most promising types of these materials at the atomic and electronic level In addition to providing an introduction to the field the main objective of this book is to present the results of the growth and structural characterization of thermoelectric materials that are of high current interest including Mg<sub>2</sub>Si PbTe Bi<sub>1-x</sub>Sb<sub>x</sub> Bi<sub>2</sub>Te<sub>3</sub> Sb<sub>2</sub>Te<sub>3</sub> Sn<sub>1-x</sub>GexTe and InSb

**Structure Determination by X-Ray Crystallography** Marcus Frederick Charles Ladd, Rex A. Palmer, 2003-09-30 This book is an account of crystal symmetry and optical and x ray diffraction techniques for examining single crystals It includes the solution of crystal structures by the current methods worked examples of crystal structure determination problems and solutions for each chapter *Structure and Performance of Cements* P. Barnes, J. Bensted, 2002-11-01 Drawing together a multinational team of authors this second edition of *Structure and Performance of Cements* highlights the latest global advances in the field of cement technology Three broad categories are covered basic materials and methods cement extenders and techniques of examination Within these categories consideration has been given Combined Analysis Daniel Chateigner, 2013-03-04 This book introduces and details the key facets of Combined Analysis an x ray and or neutron scattering methodology which combines structural textural stress microstructural phase layer or other relevant variable or property analyses in a single approach The author starts with basic theories related to diffraction by polycrystals and some of the most common combined analysis instrumental set ups are detailed Powder diffraction data treatment is introduced and in particular the Rietveld analysis is discussed The book also addresses automatic phase indexing a necessary step to solve a structure ab initio Since its effect prevails on real samples where textures are often stabilized quantitative texture analysis is also detailed Also discussed are microstructures of powder diffraction profiles quantitative phase analysis from the Rietveld analysis residual stress analysis for isotropic and anisotropic materials specular x ray reflectivity and the various associated

models Finally the book introduces the combined analysis concept showing how it is superior to the view presented when we look at only one part of the analyses This book shows that the existence of texture in a specimen can be envisaged as a way to decouple ordinarily strongly correlated parameters as measured for instance in powder diagrams and to examine and detail deeper material characterizations in a single methodology

**Handbook On Big Data And Machine Learning In The Physical Sciences (In 2 Volumes)** ,2020-03-10 This compendium provides a comprehensive collection of the emergent applications of big data machine learning and artificial intelligence technologies to present day physical sciences ranging from materials theory and imaging to predictive synthesis and automated research This area of research is among the most rapidly developing in the last several years in areas spanning materials science chemistry and condensed matter physics Written by world renowned researchers the compilation of two authoritative volumes provides a distinct summary of the modern advances in instrument driven data generation and analytics establishing the links between the big data and predictive theories and outlining the emerging field of data and physics driven predictive and autonomous systems



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