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Rietveld Refinement Practical Powder Diffraction Pattern Analysis using TOPAS. By Robert E. Dinnebier, Andreas Leineweber and John S. O. Evans. De Gruyter, 2019. Pp. 331. Price (paperback) EUR 69.95, USD 80.99, GBP 63.50. ISBN 978-3-11-045621-9, e-ISBN (PDF) 978-3-11-046138-1.

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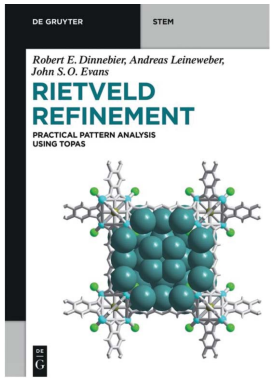
The powder diffraction method was developed over a century ago (Debye & Scherrer, 1916*a*,*b*,*c*); however, for the first 50 years, its use in science was limited, as it was viewed as information deficient. During data collection, the three-dimensional reciprocal space collapses onto the one-dimensional 2θ axis of the powder pattern, causing accidental and systematic peak overlap that reduces the amount of measured information. In 1969, Hugo Rietveld developed a strategy to circumvent this problem by modelling the whole powder pattern with a set of parameters that are refined to minimize the difference between the calculated and experimental data (Rietveld, 1969). This strategy became known as Rietveld refinement and shone a bright new light on the powder diffraction method. Ever since, the method has been used to study the crystal structure, microstructure and local structure of materials, and it provides a valuable alternative to single-crystal diffraction when crystals of suitable size and shape are not available. This book by Dinnebier, Leineweber and Evans is an excellent read about this cornerstone method of crystallography. The authors present the power of the powder diffraction technique with practical examples of data analysis using *TOPAS* (Coelho, 2018). *TOPAS* is a robust crystallographic software program that allows for the introduction of user-defined macros, tailor-made for specific data analyses. The authors explain how to use the macro language to extract the maximum amount of structural information from a diffraction pattern. Foremost, I would like to caution the reader not to be misled into believing that the book is a mere manual for the *TOPAS* software. The book masterfully and methodically covers the most important modern applications of the powder diffraction method. The authors chose to use the scripting language of *TOPAS* for the examples and case studies; however, I am convinced that the book will also serve users of other software packages and readers interested in the fundamentals of the powder diffraction method. The breadth of scope of the book becomes obvious after just a glance at its contents, which are as follows:



The fundamentals of the powder diffraction method are covered in chapter 1, followed by a discussion of the basics of Rietveld refinement in chapter 2. These chapters are written concisely, yet they contain astonishing crystallographic depth. To cater to a broader readership, the authors have kept the level of mathematics at a minimum; for the interested reader, however, they provide an appendix in chapter 13 with the basics of the higher-level mathematical machinery. These chapters give the reader a fundamental knowledge of the methods, which is necessary to understand the remaining material in the book. I enjoyed the scientific rigour in these fundamental chapters, and I also recommend them as textbook material in graduate crystallography classes.

In chapter 3, the authors describe three methods of structure-independent fitting – constrained single-peak fitting, the Le Bail method (Le Bail, 2005) and the Pawley method (Pawley, 1981) – which can be used to obtain initial values for the parameters in the Rietveld refinement. In chapter 4, they provide an account of the measured peak shapes and broadening, explaining the inevitable contributions from the instrument and the sample's microstructure. I believe these two chapters are exceptionally important, as a successful Rietveld refinement demands good starting parameters for peak positions, peak profile and background. In these chapters, the reader can learn how to properly determine and describe the starting parameters in the program and initiate Rietveld refinement.

Having covered the fundamentals, the authors continue with chapters on practical applications of the Rietveld method. In chapter 5, they discuss the quantitative phase analysis (QPA) of materials. The information provided in this chapter could be very useful for various industries that routinely perform QPA on multiphase crystalline mixtures (that can be with or without amorphous contribution). The authors then move on to focus on another important application of the powder diffraction method: crystal structure solution. It is well known that the ratio between the number of experimentally observed intensities in the diffraction pattern and the refined structural parameters is usually low, challenging the crystal structure solution process. Therefore, in chapter 6, the authors provide a comprehensive discussion of various strategies used to reduce the number of parameters in order to facilitate the solution process and stabilize the refinement. This is exemplified by the introduction of constraints, restraints, penalties and rigid bodies. Finally, in chapter 7, the authors showcase the process of crystal structure solution from powder diffraction data, using the real-space method of simulated annealing followed by whole-pattern Rietveld refinement.

In the remaining chapters, the authors focus on more advanced (and, dare I say, more exotic) applications of powder diffraction and the Rietveld method. Chapter 8 explains a strategy to analyse symmetry-lowering phase transitions by symmetry-adapted distortion mode refinement. Chapter 9 discusses the interactions of neutrons with magnetic moments, which can be successfully used to determine the magnetic structure of materials. Chapter 10 provides viable solutions for treating and analysing stacking faults and disorder in crystal structures. Chapter 11 presents an approach for the simultaneous (and synergetic) analysis of the extended structure and local structure of materials by Rietveld refinement and pair distribution function (PDF) analyses, respectively. Finally, chapter 12 explains strategies for simultaneous analyses of multiple data sets, known as parametric Rietveld refinement, which can be exceptionally useful in extracting noncrystallographic information from *in situ* collected diffraction patterns.

Each chapter is independent of the others and can be used as a stand-alone text. Even though the text is written by three authors, there is an immaculate uniformity of style. Conveniently, various input files and data sets for the examples in the book can be found online, free of charge, on the *TOPAS Wiki* page http://topas.dur.ac.uk/topaswiki/doku.php?id=book.

To the best of my knowledge, it has been over a quarter of a century since the publication of the last textbook devoted to Rietveld refinement (Young, 1993). Since then, the method has evolved and its applications have been extended to different fields. Dinnebier, Leineweber and Evans have done an outstanding job of explaining the fundamentals of the method and summarizing the exciting new developments. With this book, the reader can find answers to two questions: what information is stored in a powder diffraction pattern, and how to extract that information using *TOPAS*. I particularly like this combination of theory and practice and I wholeheartedly recommend this excellent read to any user of the powder diffraction method.

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