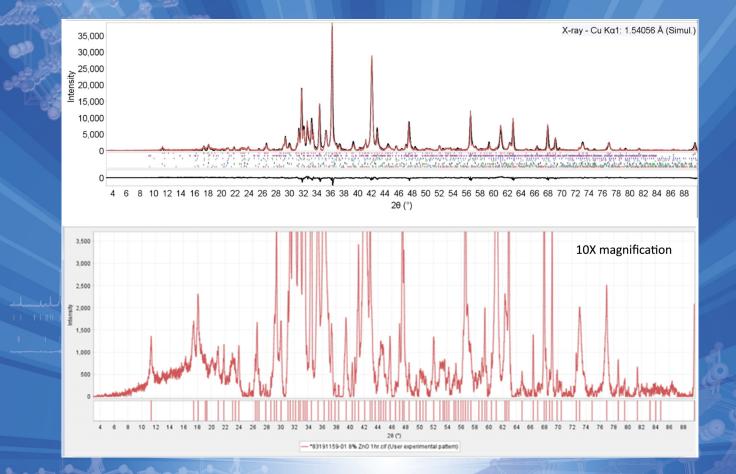
Powder Diffraction PDJ Journal of Materials Characterization



Volume 38 / Number 02 / June 2023



Powder Diffraction

Journal of Materials Characterization

Journal of the International Centre for Diffraction Data https://www.cambridge.org/core/journals/powder-diffraction Volume 38, Issues 1-4

eISSN: 1945-7413; ISSN: 0885-7156

Editor-in-Chief

Camden Hubbard, Applied Diffraction Services, USA

Managing Editor

Nicole Ernst Boris, International Centre for Diffraction Data, USA

Editors for New Diffraction Data

Stacy Gates-Rector, International Centre for Diffraction Data, USA Soorya Kabekkodu, International Centre for Diffraction Data, USA

Associate Editor for New Diffraction Data

Frank Rotella, Argonne National Laboratory (Retired), USA

Editors

Xiaolong Chen, Institute of Physics, Chinese Academy of Sciences, China José Miguel Delgado, Universidad de Los Andes, Venezuela Norberto Masciocchi, Università dell'Insubria, Italy

Editors for Crystallography Education

James Kaduk, Poly Crystallography Inc., USA Brian H. Toby, Argonne National Laboratory, USA

International Reports Editor

Winnie Wong-Ng, National Institute of Standards and Technology, USA

Calendar of Meetings and Workshops Editor

Gang Wang, Chinese Academy of Sciences, China

Advisory Board

Evgeny Antipov, Moscow State University, Russian Federation Xiaolong Chen, Chinese Academy of Sciences, China Jose Miguel Delgado, University de Los Andes, Venezuela Steve Hillier, The James Hutton Institute, UK Takashi Ida, Nagoya Institute of Technology, Japan Matteo Leoni, University of Trento, Italy Vanessa Peterson, Australian Nuclear Science and Technology Organisation, Australia Mark Rodriguez, Sandia National Labs, USA T.N. Guru Row, Indian Institute of Science, India Allison Keene, Cambridge University Press, USA

Information about editors and editorial board members correct as of 1st January 2022. For the latest information please see https://www.cambridge.org/ core/journals/powder-diffraction/information/editorial-board

Aims & Scope

ICDD's quarterly, and special topical issue, international journal, *Powder Diffraction*, focuses on materials characterization employing X-ray powder diffraction and related techniques. With feature articles covering a wide range of applications, from mineral analysis to epitactic growth of thin films to advances in application software and hardware, this journal offers a wide range of practical applications. ICDD, in collaboration with the Denver X-ray Conference Organizing Committee, has increased services for the subscribers of Powder Diffraction and authors of Advances in X-ray Analysis. Beginning in 2006, ICDD offered a copy of the previous year's edition of AXA to Powder Diffraction institutional subscribers who receive both print and on-line versions. This effectively doubles the number of articles annually available to Powder Diffraction subscribers and significantly increases the circulation for the authors in Advances in X-ray Analysis.

Subject coverage includes:

- Techniques and procedures in X-ray powder diffractometry
- Advances in instrumentation
- Study of materials including organic materials, minerals, metals and thin film superconductors
- Publication of powder data on new materials

International Centre for Diffraction Data

The International Centre for Diffraction Data ($ICDD^{(R)}$) is a non-profit scientific organization dedicated to collecting, editing, publishing, and distributing powder diffraction data for the identification of materials. The membership of the ICDD consists of worldwide representation from academe, government, and industry.

© International Centre for Diffraction Data

Published by Cambridge University Press.





Volume 38 Number 2 June 2023

Powder Diffraction

TECHNICAL ARTICLE

den exp	der X-ray diffraction intensities of corundum calculated by conventional and sity functional theory methods and extracted by deconvolutional treatment on erimental data 10.1017/S0885715623000131	81
doi:	10.101//\$0885/15623000131	

PROCEEDINGS PAPERS

Mark A. Rodriguez, John Krukar, Nichole R. Valdez, James Z. Harris, Kathryn A. Perkins, Christopher DiAntonio and Pin Yang	Evaluating the pressure dependence of PZT structures using a virtual reality environment doi:10.1017/S0885715623000143	90
Pamela S. Whitfield	Low-temperature crystal structures of the solvent dimethyl carbonate doi:10.1017/S088571562300009X	100
M. Witte	Measurement of coating thickness with X-ray diffraction doi:10.1017/S088571562300012X	112
Jessica E. Lyza, Timothy G. Fawcett, Sarah N. Page and Kelly L. Cook	Challenges of quantitative phase analysis of iron and steel slags: a look at sample complexity doi:10.1017/S0885715623000179	119

INSTRUMENTATION, ANALYSIS AND LABORATORY DEVELOPMENTS

Wolfgang Wisniewski,	Experimental evidence concerning the significant information depth of X-ray	139
Cécile Genevois,	diffraction (XRD) in the Bragg-Brentano configuration	
Emmanuel Veron and	doi:10.1017/S0885715623000052	
Mathieu Allix		

NEW DIFFRACTION DATA

James A. Kaduk, Anja Vieira Dosen and Thomas N. Blanton	Crystal structure of encorafenib, $C_{22}H_{27}ClFN_7O_4S$ doi:10.1017/S0885715623000118	145
Jose L. Pinto, Hernando Camargo and Nelson J. Castellanos	Synthesis and X-ray diffraction data of dichloro-dioxido-(4,4'-dimethyl-2,2'-bipyridyl) molybdenum (VI) doi:10.1017/S0885715623000040	152

DATA REPORTS

Massimo Zampieri,	X-ray powder diffraction data for ESP15228, C ₁₉ H ₃₄ O ₅ , a bempedoic acid metabolite	158
Guseppe Barreca and	doi:10.1017/S0885715623000106	
Norberto Masciocchi		

CALENDARS OF MEETINGS, SHORT COURSES AND WORKSHOPS

Gang Wang	Calendar of Forthcoming Meetings doi:10.1017/S0885715623000209	164
Gang Wang	Calendar of Short Courses and Workshops doi:10.1017/S0885715623000210	165

On the Cover: The cover figure was prepared from data from the manuscript "Challenges of Quantitative Phase Analysis of Iron and Steel Slags: A Look at Sample Complexity" by J.E. Lyza, T.G. Fawcett, S.N. Page, and K.L. Cook. The upper figure shows a PXRD pattern for an Electric Arc Furnace (EAF) slag while the lower figure shows the same data revealing the many minor diffraction peaks. The authors found that for various slags the number of phases present could be as many as 15 to 20, many of which are solid solutions and some exhibiting preferred orientation.

The number of phases and solid solutions of iron and steel slags present many complexities limiting successful quantitative phase analysis by PXRD methods. This manuscript shows in considerable detail that by thoroughly addressing the multiple analytical challenges that QXRD phase analysis can be successful.

Enjoy reading this manuscript by Jessica Lyza, Timothy Fawcett, Sarah Page, and Kelly Cook. The authors have clearly shown that by careful consideration of the "best" reference patterns, obtaining high quality experimental data, and addressing crystallite size and preferred orientation that the complex slag phase analysis can be successfully performed for samples with 10–20 phases.



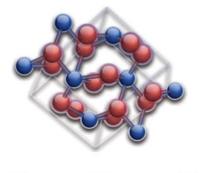
WORKING TOGETHER FOR YOU

With 1,000,000+ patterns available at your fingertips, ICDD's PDF® databases and MDI's JADE[®] software work together to make your life easier. Let the software work for the science and take your results further.



ABOUT US

For over 30 years, The ICDD and MDI have worked together in a complementary manner since MDI began in 1987. The XRD community has trusted MDI to provide unbiased results and help interpret both the everyday and the difficult XRD data. We are proud of our products and the daily effort we put forth towards advancing the science of XRD. Materials Data creates XRD software applications to collect, analyze, and simulate XRD data. These products are here to help solve issues in an enormous array of materials science projects, and may be found in labs around the world with data collected on virtually every brand of XRD equipment.



► @TheICDD **f** @TheICDD

OUR 2023 PRODUCTS

PDF-4+

Phase Identification and Quantitation The world's largest sources of inorganic diffraction data from crystals and powders in a single database featuring 480,300+ entries, including 369,500+ entries with atomic coordinates.



PDF-4+/Web

Provides portability to the PDF-4+ database via the internet.

PDF-4/Axiom

Quality Plus Value

Phase identification and quantitation that requires diffraction equipment manufacturer or vendor software.

PDF-2



Phase Identification + Value Quality and subfile filters combined with 71 different searches and 57 display fields enable you to target your results for more accurate identification.

PDF-4/Organics Solve Difficult Problems, Get Better Results Designed to solve difficult problems that are analyzed by powder diffraction analysis for a multitude of applications in the pharmaceutical, regulatory, specialty chemical, biomaterial, and forensic fields.

PDF-4/Minerals

Comprehensive Mineral Collection Ninety-seven percent of all known mineral types, as defined by the International Mineralogical Association (IMA), are represented in the database, as well as many unclassified minerals.



🥑 @ICDDICDD

JADE Pro JADE Works The Way You Do

Automate your analysis with JADE. In so many cases, it's just one click and you're done. Often these results are better than those an experienced analyst could report and in a more timely manner.

For more information contact ICDD at marketing@icdd.com

@ThelCDD

ICDD, the ICDD logo, PDF, Materials Data, JADE, Denver X-ray Conference, Denver X-ray Conference logo, and Materials Data-JADE-SM-WPF logo are registered in the U.S. Patent and Trademark Office. Powder Diffraction File, MDI, and the MDI-Materials Data logo are trademarks of the JCPDS-International Centre for Diffraction Data. ©2022 JCPDS-International Centre for Diffraction Data

LET OUR TEAM OF EXPERTS HELP YOU TAKE YOUR SKILLS TO THE NEXT LEVEL!





For the novice with some XRD knowledge or for the experienced with an interest in the theory behind XRD, this clinic offers a strong base for increased lab performance.

The clinic covers instrumentation, specimen preparation, data acquisition and qualitative phase analysis through live demonstrations. It also covers hands-on use of personal computers for demonstration of the latest software including data mining with the Powder Diffraction File (PDF) and use of the powder diffractometer: optical arrangement, factors affecting instrumentation profile width, choice and function of divergence slit, calibration and alignment, detectors, and X-ray optics.

www.icdd.com/xrd

Advanced Methods in X-ray Powder Diffraction Clinic:

For the experienced XRD scientist, this session offers enhanced analysis skills through intense problem solving, as well as an introduction to the Rietveld Method. The course emphasizes computer-based methods of data interpretation, both for qualitative and quantitative phase analysis.

The advanced course covers a wide range of topics including systematic errors, factors affecting intensities of diffraction peaks; data reduction algorithms; phase identification; advanced data mining with the PDF and its application in search/match; powder pattern indexing methods; structure solution methods; quantitative phase analysis using both reference intensity ratio (RIR) and Rietveld Method.



Rietveld Refinement & Indexing Clinic:

Powder pattern indexing and Rietveld structural refinement techniques are complementary and are often combined to determine the structure of a material. Successful indexing of a powder pattern is considered strong evidence for phase purity. Indexing is considered a prelude to determining the crystal structure, and permits phase identification by lattice matching techniques. This clinic introduces the theory and formalisms of various indexing methods and structural refinement techniques along with quantitative analysis. One unique aspect of this clinic is the extensive use of computer laboratory problem solving and exercises that teach method development in a hands-on environment.

www.icdd.com/rietveld

Practical X-ray Fluorescence Clinic:

From theory to hands-on exercises, this course offers techniques and skills to improve lab performance. Discover the latest in cutting-edge instruments such as TXRF, hand-held devices, energy dispersive and wavelength dispersive spectrometers through live demonstrations.

The XRF course covers the basics of X-ray spectra; instrumentation design; methods of qualitative and quantitative analysis; specimen preparation and applications for both wavelength and energy dispersive spectrometry. The course emphasizes quantitative methods, use of automated X-ray spectrometers, review of mathematical matrix correction procedures, and new developments in XRF.

www.icdd.com/xrf

More information at www.icdd.com/icdd-education

8⁺ in **f**

Please note: A minimum of 10 registrants per course is required, otherwise the course will be cancelled and your registration fee will be refunded. You will be notified of a course cancellation no later than two weeks prior to the start of the course.



For More Information Contact:

Eileen Jennings, Education Coordinator Tel: 610.325.9814 Fax: 610.325.9823 Email: clinics@icdd.com

Location

ICDD Headquarters 12 Campus Boulevard Newtown Square, Pennsylvania 19073-3273 USA

@2021 JCPDS-International Centre for Diffraction Data

ICDD 07/20





GRANT-IN-AID FUNDS ARE AVAILABLE DO NOT DELAY!

Proposal Submission Deadlines 31 January and 31 July

Does your research project involve the preparation and characterization of new materials using powder diffraction techniques?

If the answer is YES, then ICDD's Grant Program is the perfect fit for you!

https://www.icdd.com/grant-in-aid

Please email sample patterns to:

Denise DelCasale ICDD Grant-in-Aid Coordinator Delcasale@icdd.com

ICDD for over *80 years* has been dedicated to collecting, editing, publishing, and distributing powder diffraction data for the identification of crystalline materials. To assist us in this growth, ICDD has called on researchers from around the world to contribute their experimental data. In return, ICDD supports their efforts by funds provided through our Grant-in-Aid Program.



ICDD's approved grantees receive these additional benefits:

- A 50% price reduction on a PDF-4+ or PDF-4/Organics product
- · Financial support to aid current research projects
- Publication of pattern(s) in the Powder Diffraction File™ (PDF[®]) once approved by the Editorial Department
- Acknowledgement of your publication in the PDF with a certificate
- First-time grantees receive a complimentary one-year subscription to *Powder Diffraction Journal*



ICDD, the KDD logo, PDF and JADE are registered in the U.S. Patient and Trademark Office. Powder Diffraction File, Materials Data, Materials Data, JADE logo, and Derver Xing: Conference logo are trademarks of the JCPDE/International Centre for Diffraction Data, 2021 JCPDE/International Centre for Diffraction Data, 2021.

https://doi.org/10.1017/S0885715623000088 Published online by Cambridge University Press