Powder Diffraction *PDJ Journal of Materials Characterization*

CrossMark

AUSTRALIAN X-RAY ANALYTICAL ASSOCIATION WORKSHOPS, CONFERENCE AND EXHIBITION

CAMBRIDGE

VERSITY PRESS Volume 32 / Supplement 2 / December 2017

5-9 FEBRUARY 2017 PULLMAN ALBERT PARK MELBOURNE, VIC, AUSTRALIA



www.axaaconference.info

Twitter: @axaa_org | #axaa2017





Powder Diffraction

An International Journal of Materials Characterization

CODEN: PODIE2 ISSN: 0885-7156

EDITORIAL

Nathan A.S. Webster and Vanessa K. Peterson	Proceedings of the 2017 Australian X-ray Analytical Association workshops, con- ference, and exhibition	S 1

TECHNICAL ARTICLES

Helen E. Maynard-Casely, Norman Booth, Leo Anderberg, Helen E.A. Brand and Daniel V. Cotton	What you see and what you get: combining near-infrared spectroscopy with powder diffraction	S3
Xiaodong Wang and Arie van Riessen	Omega–Phi compensated GID in side inclination mode for measurement of residual stress in polycrystalline thin films	S 9
Henry J Kirkwood, Martin D de Jonge, Daryl L Howard, Chris G Ryan, Grant van Riessen, Felix Hofmann, Matthew R Rowles, Anna M Paradowska and Brian Abbey	Polycrystalline materials analysis using the Maia pixelated energy-dispersive X-ray area detector	S16
Dubravka Šišak Jung, Tilman Donath, Oxana Magdysyuk and Jozef Bednarcik	High-energy X-ray applications: current status and new opportunities	S22
Mikael Larsson, Johan B. Lindén, Simarpreet Kaur, Brock Le Cerf and Ivan Kempson	Cu K-edge XANES: polymer, organic, inorganic spectra, and experimental considerations	S28
Tyron Turnbull, Michael Douglass, Eva Bezak, Benjamin Thierry and Ivan Kempson	An image processing application for quantitative cross-correlative microscopy for large cell-populations: a gold nanoparticle radiosensitisation study	S33
Matthew R. Rowles, Cheng-Cheng Wang, Kongfa Chen, Na Li, Shuai He and San-Ping Jiang	Temperature-dependent structural behaviour of samarium cobalt oxide	S38
James C. Pramudita, Vanessa K. Peterson, Justin A. Kimpton and	Potassium-ion intercalation in graphite within a potassium-ion battery examined using <i>in situ</i> X-ray diffraction	S43

Neeraj Sharma

Josie E. Auckett, A. David Dharma, Marina P. Cagnes, Tamim A. Darwish, Brendan F. Abrahams, Ravichandar Babarao, Timothy A. Hudson, Richard Robson, Keith F. White and Vanessa K. Peterson	Lattice response of the porous coordination framework Zn(hba) to guest adsorption	S49
Marie Clancy, Mark J. Styles, Colleen J. Bettles, Nick Birbilis, Justin A. Kimpton and Nathan A. S. Webster	In situ XRD investigation of the evolution of surface layers on Pb-alloy anodes	S54
Chee W. Loy, Khamirul A. Matori, Norhazlin Zainuddin, Andrew E. Whitten, Christine Rehm, Liliana de Campo, Anna Sokolova and Siegbert Schmid	Crystallographic characterization of fluorapatite glass-ceramics synthesized from industrial waste	S61
Nathan A.S. Webster, Mark I. Pownceby, Natalie Ware and Rachel Pattel	Predicting iron ore sinter strength through partial least square regression (PLSR) analysis of X-ray diffraction patterns	S66
Adijat T. Awoniran, Annelly Ketheson, Sandra Piazolo and Damian B. Gore	Legacy base metal slags can generate toxic leachates	S70
Jian Li, Laura Kuhar, Peter Austin and Micheal Da Costa	Characterization of a low-grade copper-sulphide ore to assess its suitability for <i>in situ</i> recovery	S78
Nathan A. S. Webster, Mark I. Pownceby and Rachel Pattel	Fundamentals of silico-ferrite of calcium and aluminium (SFCA) and SFCA-I iron ore sinter bonding phase formation: effects of mill scale addition	S85
D. B. Gore, M. Choat, D. E. Jacob and G. Gloy	Which elements are useful for understanding the composition of ancient papyrus inks?	S90
Christopher E. Marjo, Gillan Davis, Bin Gong and Damian B. Gore	Spatial variability of elements in ancient Greek (ca. 600–250 BC) silver coins using scanning electron microscopy with energy dispersive spectrometry (SEM-EDS) and time of flight-secondary ion mass spectrometry (ToF-SIMS)	S95

Powder Diffraction

An International Journal of Materials Characterization

Editor-in-Chief

Camden Hubbard Applied Diffraction Services 110 Crestview Lane Oak Ridge, Tennessee 37830, U.S.A. camden.hubbard@me.com

Managing Editor

Nicole M. Ernst Boris International Centre for Diffraction Data 12 Campus Boulevard Newtown Square, Pennsylvania 19073-3273, U.S.A. boris @icdd.com

Editor for New Diffraction Data

Soorya Kabekkodu International Centre for Diffraction Data 12 Campus Boulevard Newtown Square, Pennsylvania 19073-3273, U.S.A. kabekkodu@icdd.com

Associate Editor for New Diffraction Data

Stacy Gates-Rector International Centre for Diffraction Data 12 Campus Boulevard Newtown Square, PA 19073-3273, U.S.A. gates-rector@icdd.com

Editors

Xiaolong Chen Institute of Physics Chinese Academy of Sciences No. 8 Nansanjie, Zhongguancun, Haidian District, Beijing 100190, China xlchen@iphy.ac.cn

José Miguel Delgado Universidad de Los Andes Facultad de Ciencias Departamento de Química Lab. de Cristalografía Mérida 5101 Venezuela migueld@ula.ve

Norberto Masciocchi Universitá dell'Insubria Dipartimento di Scienza e Alta Tecnologia via Valleggio 11 Como 22100 Italy norberto.masciocchi@uninsubria.it

Editors for Crystallography Education

James Kaduk Poly Crystallography Inc. 423 East Chicago Avenue Naperville, Illinois 60540-5407, U.S.A. Kaduk@polycrystallography.com

Brian H. Toby Argonne National Laboratory Advanced Photon Source 9700 S. Cass Ave., Bldg. 401/B4192, Argonne, Illinois 60439-4856, U.S.A. brian.toby@anl.gov

International Reports Editor

Winnie Wong-Ng Materials Measurement Science Division National Institute of Standards and Technology 100 Bureau Drive, Mail Stop 8520 Gaithersburg, MD 20899-8520, U.S.A. winnie.wong-ng@nist.gov

Calendar of Meetings and Workshops Editor

Gang Wang Institute of Physics Chinese Academy of Sciences No. 8 Nansanjie, Zhongguancun, Haidian District, Beijing 100190, China gangwang@iphy.ac.cn

On the Cover: View of the Melbourne skyline from the parkland next to where AXAA-2017 was held.

Powder Diffraction is a quarterly journal published by the JCPDS-International Centre for Diffraction Data through Cambridge University Press.

Powder Diffraction is a journal of practical technique, publishing articles relating to the widest range of application—from materials analysis to epitactic growth of thin films and to the latest advances in software. Although practice will be emphasized, theory will not be neglected, especially as its discussion will relate to better understanding of technique.

Submit manuscripts online at http://mc.manuscriptcentral.com/pdj. See the instructions on submitting your manuscript linked on that page. The editors will consider all manuscripts received, but assume no responsibility regarding them. There is no publication charge.

Most proofs are handled via email at ztokushige@cambridge.org. Please include the job number in all correspondence.

For advertising rates and schedules contact M.J. Mrvica Associates, 2 West Taunton Avenue, Berlin, NJ 08009; Phone: 856-768-9360; Fax: 856-753-0064; Email: mjmrvica@mrvica.com

& Online Online
\$133
£83
\$35
\$271

Subscription rates to Eastern Hemisphere include air freight service.

Back-Number Prices. 2017 single copies: \$129.

Subscription, renewals, and address changes should be addressed to Subscription Fulfillment, *Powder Diffraction*, Cambridge University Press, One Liberty Plaza, 20th floor New York, NY 10006-1435 (for U.S.A., Canada, and Mexico); or Cambridge University Press, The Edinburgh Building, Shaftsbury Road, Cambridge, CB2 8RU, Cambridge, England (for UK and elsewhere). Allow at least six weeks advance notice. For address changes please send both old and new addresses and, if possible, include a mailing label from the wrapper of a recent issue.

Claims, Single Copy Replacement, Back Volumes, and Reprints: Missing issue requests will be honored only if received within six months of publication date (nine months for Australia and Asia). Single copies of a journal may be ordered and back volumes are available in print or microform. Individual subscribers please contact Subscription Fulfillment, *Powder Diffraction*, One Liberty Plaza, 20th floor New York, NY 10006-1435. Phone: 845-353-7500; Toll free: 800-872-7423; Fax: 845-353-4141. Email: subscriptions_newyork@cambridge.org.

Powder Diffraction (ISSN: 0885-7156) is published quarterly (4X annually) by the JCPDS-International Centre for Diffraction Data through One Liberty Plaza, 20th floor New York, NY 10006-1435. POSTMASTER: Send address changes to *Powder Diffraction*, One Liberty Plaza, 20th floor New York, NY 10006-1435, USA. Periodicals postage paid in New York, NY and additional mailing offices.

Permission for Other Use: Permission is granted to quote from the journal with the customary acknowledgment of the source. To reprint a figure, table, or other excerpt requires the consent of one of the authors and notification to Cambridge University Press.

Requests for Permission: No part of this publication may be reproduced in any forms or by any means, electronic, photocopying, or otherwise, without permission in writing from Cambridge University Press. Policies, request forms, and contacts are available at: http://www.cambridge.org/about-us/rights-permissions/. Permission to copy (for users in the U.S.A.) is available from Copyright Clearance Center: http://www.copyright.com. Email: info@copyright.com.

Document Delivery and Online Availability: Abstracts of journal articles published by Cambridge University Press are available from Cambridge Core (https://www.cambridge.org/pdj).

Copyright © 2017 JCPDS- International Centre for Diffraction Data, 12 Campus Blvd., Newtown Square, PA 19073-3273, U.S.A. All rights reserved. www.icdd. com/products/journals.htm

Diffraction Data You Can Trust

ICDD databases are the only crystallographic databases in the world with quality marks and quality review processes that are ISO certified.



Targeted For Material Identification and Characterization

www.icdd.com/products/pdf4.htm



www.icdd.com | marketing@icdd.com ICDD, the ICDD logo and PDF are registered in the U.S. Patent and Trademark of ICPDS - International Centre for Diffraction Data - 6/17 Powder Diffraction File is a trademark of JCPDS - International Centre for Diffraction Data - 6/17

8⁺ in f E