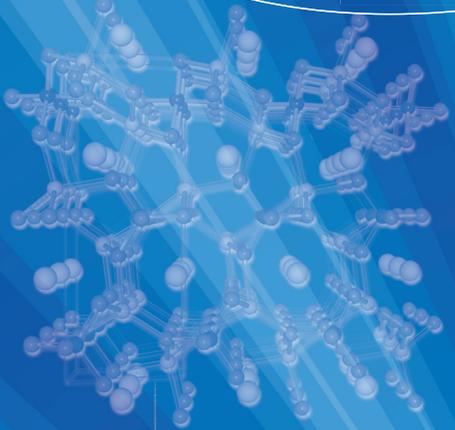




# Powder Diffraction PDJ

JOURNAL OF MATERIALS CHARACTERIZATION



SE

BSE

FSE

tilt 70°

BSE

EDX

SE

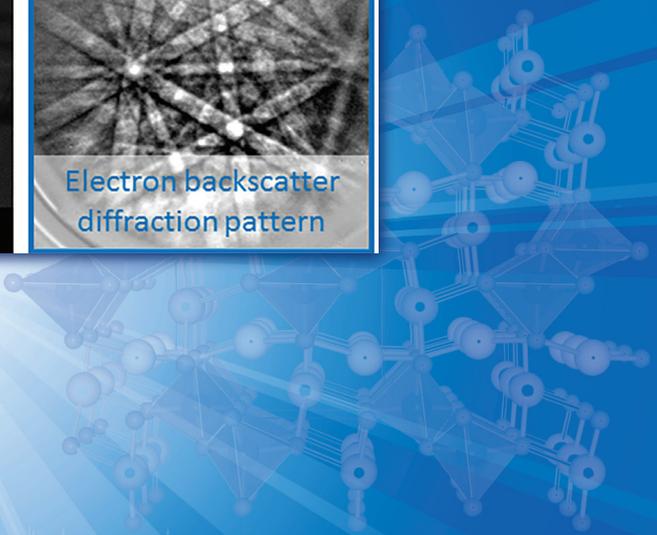
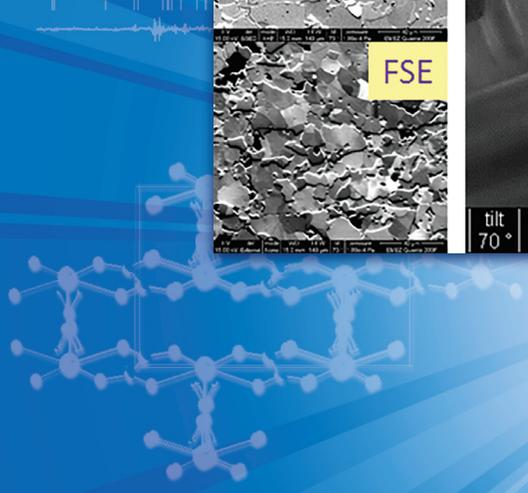
EBSD

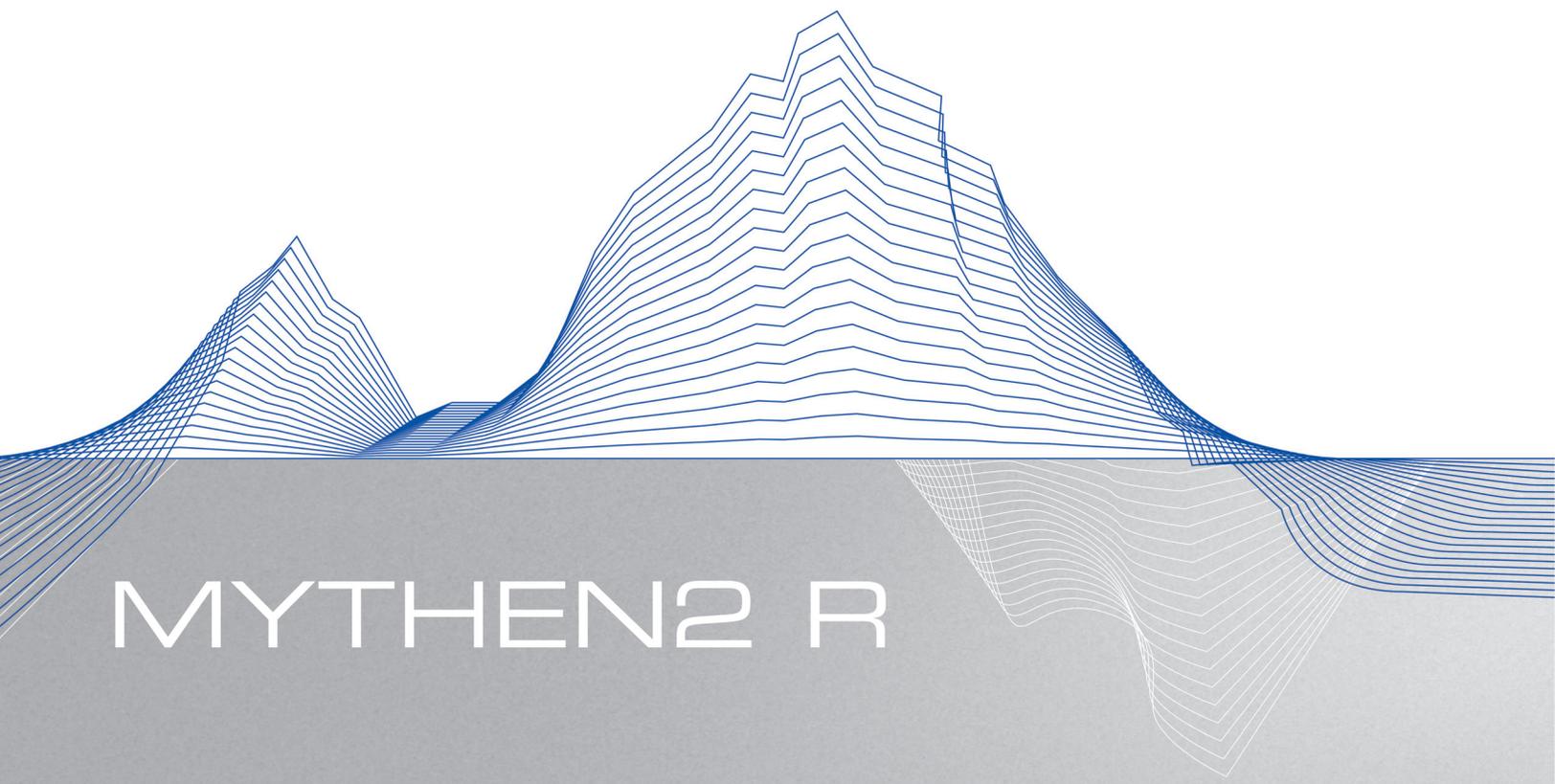
FSE

sample

EDX spectrum

Electron backscatter diffraction pattern





## MYTHEN2 R



### *Microstrip Hybrid Photon Counting X-ray Detector Series*

*Top performance in all high-throughput  
applications*

- *Noise-free single-photon counting  
from Ti to Ag radiation*
- *Compact design fits in any  
diffractometer*
- *640- and 1280-strip modules*
- *Multi-modular systems for the  
laboratory*

*laboratory and industry*

## EDITORIALS

Camden Hubbard	Excited to be Editor-in-Chief for <i>Powder Diffraction</i>	89
Tom Blanton	Proceedings for the 14th European Powder Diffraction Conference published online as a 2015 Special Supplement Issue of Powder Diffraction Journal	90
Tom Blanton and Lora Brehm	Sixty-third Denver X-ray Conference and selected Advances in X-ray Analysis papers for the June <i>Powder Diffraction</i> issue	92

## TECHNICAL ARTICLES

J. Prost, P. Wobrauschek and C. Strelt	Comparison of different excitation modes for the analysis of light elements with a TXRF vacuum chamber	93
Conal E. Murray, Jean L. Jordan-Sweet, Stephen W. Bedell and E. Todd Ryan	Stress determination through diffraction: establishing the link between Kröner and Voigt/Reuss limits	99
Karsten Kunze	Crystal orientation measurements using SEM–EBSD under unconventional conditions	104
Kouichi Tsuji, Atsushi Tabe, Peter Wobrauschek and Christina Strelt	Secondary excitation process for quantitative confocal 3D-XRF analysis	109
Minoru Inoue, Yasujiro Yamada, Mao Kitamura, Norifumi Gotoh, Naoki Kawahara and Michael Mantler	A new methodical approach based on Compton scattering and XRF: quantitative analysis of CO <sub>2</sub> and loss on ignition in quicklime	113
Z. N. Guo, B. L. Han, P. Li, H. H. Zhang and W. X. Yuan	Solid solubility and superconductivity of Fe <sub>y</sub> Te <sub>1-x</sub> X <sub>x</sub> (X = Se, S)	117
Giovanni Cavallo, Maria Pia Riccardi and Roberto Zorzin	Powder diffraction of yellow and red natural earths from Lessini Mountains in NE Italy	122
A. Le Bail and L'. Smrčok	Face-sharing octahedra in Cs <sub>3</sub> Al <sub>2</sub> F <sub>9</sub> and Cs <sub>2</sub> AlF <sub>5</sub>	130
W. Wong-Ng, G. Liu, Y. Yan, K. R. Talley and J. A. Kaduk	X-ray powder diffraction studies of (Ba <sub>x</sub> Sr <sub>1-x</sub> ) <sub>2</sub> Co <sub>2</sub> Fe <sub>12</sub> O <sub>22</sub> and (Ba <sub>x</sub> Sr <sub>1-x</sub> )Co <sub>2</sub> Fe <sub>16</sub> O <sub>27</sub>	139
A. Dominic Fortes	X-ray powder diffraction analysis of two new magnesium selenate hydrates, MgSeO <sub>4</sub> ·9H <sub>2</sub> O and MgSeO <sub>4</sub> ·11H <sub>2</sub> O	149
James A. Kaduk, Kai Zhong, Thomas N. Blanton and Stacy Gates	Crystal structure of levalbuterol hydrochloride polymorph A (Xopenex), C <sub>13</sub> H <sub>22</sub> NO <sub>3</sub> Cl	158
D. Y. Leshok, N. N. Golovnev and S. D. Kirik	Cystamindi-ium tetrachlorocuprate [NH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> SS(CH <sub>2</sub> ) <sub>2</sub> NH <sub>3</sub> ][CuCl <sub>4</sub> ]: synthesis, crystal structure, and thermal decomposition	163
James A. Kaduk, Kai Zhong and Thomas N. Blanton	Crystal structure of rilpivirine, C <sub>22</sub> H <sub>18</sub> N <sub>6</sub>	170

## NEW DIFFRACTION DATA

XiaoLi Ma, PeiXiao Tang, Jin Yan, XiaoQing Wu, Qiang Chen and Hui Li	X-ray powder diffraction data for beta-methyl vinyl phosphate (C <sub>29</sub> H <sub>27</sub> N <sub>2</sub> O <sub>10</sub> P)	175
Gerzon E. Delgado, Asiloé J. Mora, Jines E. Contreras and Cecilia Chacón	X-ray powder diffraction data for 1-methylhydantoin, an antiasthmatic and antidepressive hydantoin compound	178
R. Pažout, J. Maixner and V. Bartůněk	X-ray powder diffraction data for lanthanum trilactate trihydrate	182
Jing Wang, Di Wu, Shan Shan Li, Pei Xiao Tang, Li Li Wang and Hui Li	X-ray powder diffraction data for calcium(II)-naproxen complex (C <sub>28</sub> H <sub>26</sub> CaO <sub>6</sub> ·2H <sub>2</sub> O)	185

## CALENDARS

Gang Wang	Calendar of Forthcoming Meetings <i>Powder Diffraction June 2015</i>	188
Gang Wang	Calendar of Short Courses & Workshops <i>Powder Diffraction June 2015</i>	190

# 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

## 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  
miguel@ula.ve

Norberto Masciocchi  
Università 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: Setup of an analytical SEM for simultaneous detection of SE, BSE, FSE imaging signals, EDX spectra and EBSD patterns from "Crystal orientation measurements using SEM-EBSD under unconventional conditions". (Courtesy of Karsten Kunze).

*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 epitaxial 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 [kdaly@cambridge.org](mailto:kdaly@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](mailto:mjmrvica@mrvica.com)

## Subscription Prices 2015

	Print & Online	Online
Individual (U.S. & Canada)	\$165	\$121
Individual (outside U.S. & Canada)	£102	£75
Student	N/A	\$30
Institutional or Library	\$300	\$199

Subscription rates to Eastern Hemisphere include air freight service.

**Back-Number Prices.** 2015 single copies: \$66.

**Subscription, renewals, and address changes** should be addressed to Subscription Fulfillment, *Powder Diffraction*, Cambridge University Press, 100 Brook Hill Drive, West Nyack, NY 10013-2113 (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*, Cambridge University Press, 100 Brook Hill Drive, West Nyack, NY 10013-2113. Phone: 845-353-7500; Toll free: 800-872-7423; Fax: 845-353-4141. Email: [subscriptions\\_newyork@cambridge.org](mailto:subscriptions_newyork@cambridge.org).

*Powder Diffraction* (ISSN: 0885-7156) is published quarterly (4X annually) by the JCPDS-International Centre for Diffraction Data through Cambridge University Press, 32 Avenue of the Americas, New York, NY 10013-2473. POSTMASTER: Send address changes to *Powder Diffraction*, Cambridge University Press, 100 Brook Hill Drive West Nyack, NY 10994-2113, 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://journals.cambridge.org/action/rightsAndPermissions>. Permission to copy (for users in the U.S.A.) is available from Copyright Clearance Center: <http://www.copyright.com>. Email: [info@copyright.com](mailto:info@copyright.com).

**Document Delivery and Online Availability:** Abstracts of journal articles published by Cambridge University Press are available from Cambridge Journals Online (<http://journals.cambridge.org/action/displayJournal?jid=PDJ>).

**Copyright © 2015 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](http://www.icdd.com/products/journals.htm)**

# Improve your Image

# G670

Imaging Plate Guinier Camera



Capillary Sample Holder

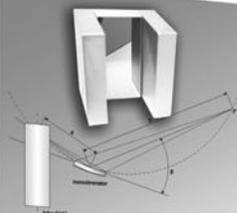


Diamond Anvil Cell Holder



Capillary Heater Device

Johansson Monochromator Crystals



Diode Laser Furnace



Low Temperature Device



Vertical Base for Liquids/Thin Films



Sample Changer

Capillary Boy



Plane Sample Holder

Your Decision for Precision



# HUBER

Diffraction and Positioning Equipment

www.xhuber.com  
info@xhuber.com



**HUBER**  
Diffraction and Positioning Equipment

Imaging Plate Guinier Camera 670  
Model No. 0670.000  
Serial No. 066  
Assembled in Germany

CE