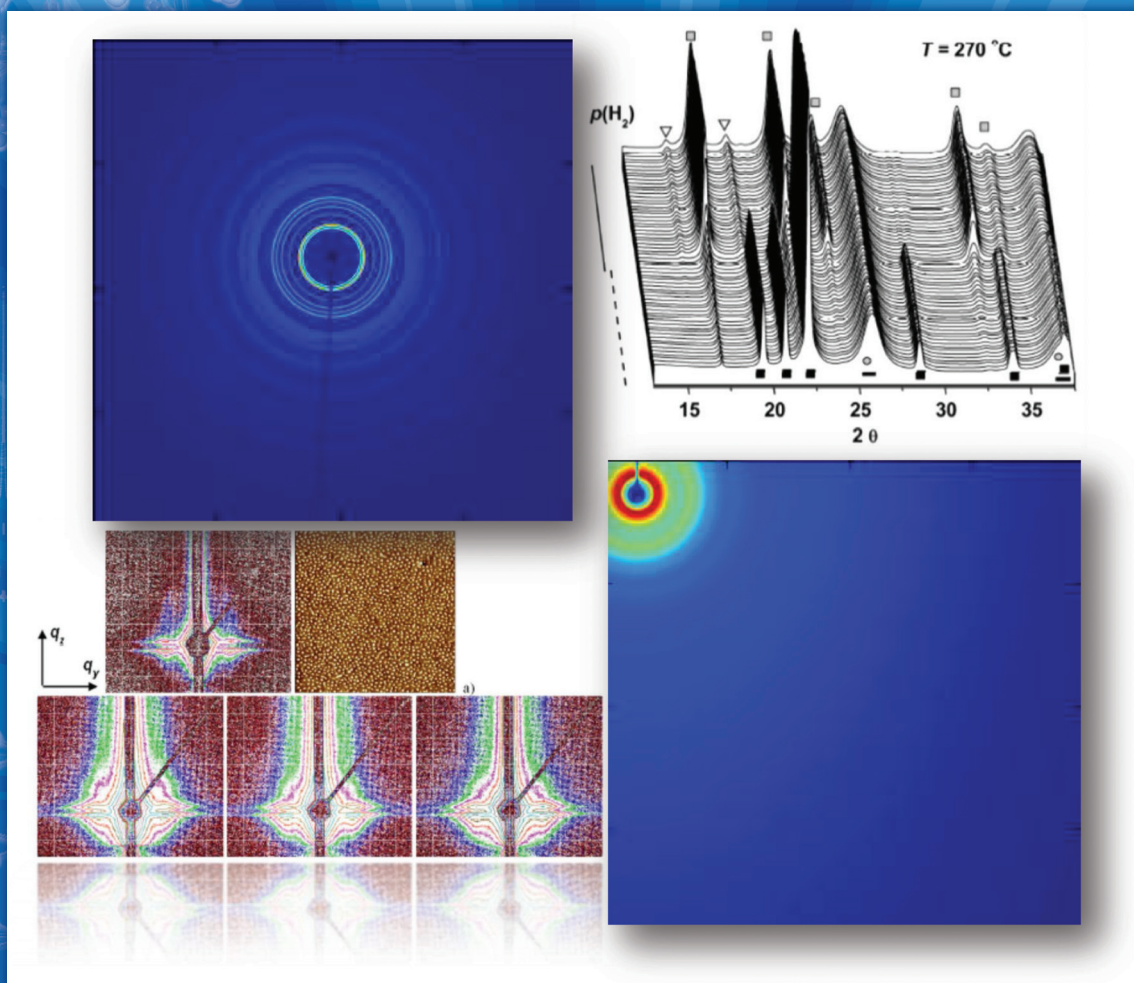


# Powder Diffraction PDJ

JOURNAL OF MATERIALS CHARACTERIZATION

EPDIC14: the European Powder Diffraction Conference, Aarhus, Denmark, 15–18 June 2014

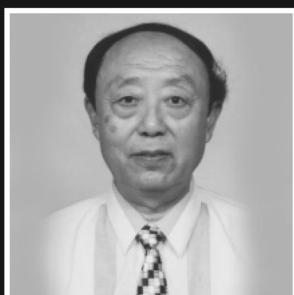


who contribute experimental powder diffraction patterns to the Powder Diffraction File

### AS A MEMBER OF THIS ELITE GROUP, YOU WILL RECEIVE THE FOLLOWING BENEFITS:

- Financial support to aid current research
- Publication of pattern(s), if accepted by the Editorial Department, in the Powder Diffraction File
- Receive calibration standards
- Purchase certain products at reduced prices
- Web-based access to the list of compounds in the ICDD master database—includes published patterns, as well as patterns still in the editorial process
- First-time grantees receive a complimentary one-year subscription to *Powder Diffraction*

### DISTINGUISHED GRANTEES



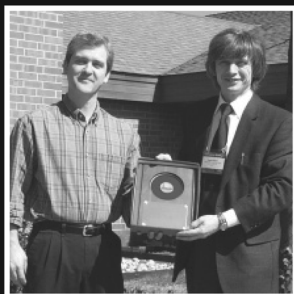
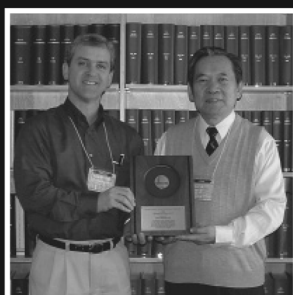
**2013: (L)**  
Professor Xinkan Yao

**2010: (R)**  
Dr. Tom Blanton  
presenting to  
Professor Bogdan Lazoryak



**2007: (L)**  
Dr. Miguel Delgado  
presenting to  
Dr. Sergei Kirik

**2004: (R)**  
Dr. Tom Blanton  
presenting to  
Professor Shao-Fan Lin



**2001: (L)**  
Dr. Tom Blanton  
presenting to  
Professor Evgeny Antipov

**1998: (R)**  
Dr. Ekkehart Tillmanns



For over 50 years, ICDD has supported a well-developed program of grants to researchers around the world.

One of our main objectives is to expand the range of reference materials by producing and cataloging high-quality X-ray diffraction patterns in our internationally renowned database, the Powder Diffraction File. Thanks to the longevity of this program, these contributions account for approximately a quarter of the current experimental file. ICDD awards financial support to qualified investigators in the form of grants-in-aid on a competitive proposal basis. The duration of a grant is 12 months with two cycles per year. Cycle I begins 1 April and Cycle II begins 1 October.

### Geographic Locations of Grants for the Past 15 Years:

Argentina	Malaysia
Austria	Netherlands
Canada	P.R. of China
Chile	Poland
Columbia	Portugal
Czech Republic	Russia
Estonia	Spain
Finland	Switzerland
France	Taiwan
Germany	Tunisia
India	Ukraine
Israel	United Kingdom
Italy	United States
Japan	Uruguay

Total Proposals Funded  
for the Past 15 Years: **720**

Could you be the next Distinguished Grantee?  
[www.icdd.com/grants](http://www.icdd.com/grants)

For more information on  
ICDD's Grant-in-Aid, visit  
[www.icdd.com/grants](http://www.icdd.com/grants)

## EDITORIAL

- Michela Brunelli,  
Paolo Scardi and  
Jens-Erik Jørgensen
- Proceedings of the 14th European Powder Diffraction Conference
- S1

## TECHNICAL ARTICLES

- Andrea Bernasconi,  
Jonathan Wright and  
Nicholas Harker
- Total scattering experiments on glass and crystalline materials at the ESRF on the ID11 Beamline
- S2
- Dmytro Korablov,  
Thomas K. Nielsen,  
Flemming Besenbacher and  
Torben R. Jensen
- Mechanism and kinetics of early transition metal hydrides, oxides, and chlorides to enhance hydrogen release and uptake properties of  $MgH_2$
- S9
- Dieter Jehnichen,  
Doris Pospiech, Peter Friedel,  
Guping He, Alessandro Sepe,  
Jianqi Zhang, Christine  
M. Papadakis, Rosa Taurino  
and Jan Perlich
- Thin-film morphologies of block copolymers with nanoparticles
- S16
- Kenneth R. Beyerlein,  
Christian Jooss, Anton Barty,  
Richard Bean,  
Sébastien Boutet, Sarnjeet  
S. Dhesi, R. Bruce Doak,  
Michael Först, Lorenzo Galli,  
Richard A. Kirian,  
Joseph Kozak, Michael Lang,  
Roman Mankowsky,  
Marc Messerschmidt, John  
C. H. Spence, Dingjie Wang,  
Uwe Weierstall, Thomas  
A. White, Garth J. Williams,  
Oleksandr Yefanov, Nadia  
A. Zatsepin, Andrea Cavalleri  
and Henry N. Chapman
- Trace phase detection and strain characterization from serial X-ray free-electron laser crystallography of a  $Pr_{0.5}Ca_{0.5}MnO_3$  powder
- S25
- B. Peplinski, C. Adam,  
B. Adamczyk, R. Müller,  
M. Michaelis, T. Krahl and  
F. Emmerling
- Nanocrystalline and stacking-disordered  $\beta$ -cristobalite  $AlPO_4$ : the now deciphered main constituent of a municipal sewage sludge ash from a full-scale incineration facility
- S31
- Dubravka Šišak Jung,  
Tomica Hrenar, Ozren Jović,  
Petra Kalinovičić and  
Ines Primožič
- Using synergy of experimental and computational techniques to solve monomer-trimer dilemma
- S36

P. Mikula and M. Vrána	New type of versatile neutron diffractometer with a double-crystal monochromator system	S41
Andrea Troian, Luca Rebuffi, Matteo Leoni and Paolo Scardi	Toward a reference material for line profile analysis	S47
M. Kučeráková, S. Vratislav, L. Kalvoda and Z. Trojanová	Analysis of preferential orientation in zirconium samples deformed by uniaxial tension using neutron and X-ray diffraction	S52
Luca Rebuffi, Paolo Scardi and Manuel Sanchez del Rio	Design and management of a powder diffraction beamline for Line Profile Analysis: a realistic ray-tracing approach	S56
Giorgia Confalonieri, Monica Dapiaggi, Marco Sommariva, Milen Gateshki, Andy N. Fitch and Andrea Bernasconi	Comparison of total scattering data from various sources: the case of a nanometric spinel	S65
Marwa Ammar, Walid Oueslati, Nejmeddine Chorfi and Abdesslem Ben Haj Amara	The water retention mechanism of a Cs <sup>+</sup> and Na <sup>+</sup> exchanged montmorillonite: effect of relative humidity and ionic radius on the interlayer	S70
Efthymios Polatidis, Nikolay Zotov and Eric J. Mittemeijer	Stress-induced phase transformations in thermally cycled superelastic NiTi alloys: <i>in situ</i> X-ray diffraction studies	S76
Zdenek Pala, Jaroslava Fojtikova, Tomas Koubsky, Radek Musalek, Josef Strasky, Jiri Capek, Jiri Kyncl, Libor Beranek and Kamil Kolarik	Study of residual stresses, microstructure, and hardness in FeB and Fe <sub>2</sub> B ultra-hard layers	S83
C. Schimpf, M. Schwarz, C. Lathe, E. Kroke and D. Rafaja	Corrugations of the basal planes in hexagonal boron nitride and their impact on the phase transition to cubic boron nitride	S90
I. O. Troyanchuk, M. V. Bushinsky, V. Efimov, S. Schorr, C. Ritter and V. Sikolenko	Ferromagnetic ordering in La <sub>0.7</sub> Sr <sub>0.3</sub> Mn <sup>3+</sup> <sub>0.85</sub> Nb <sup>5+</sup> <sub>0.15</sub> O <sub>3</sub> manganite	S97
Dina Deyneko, Sergey Stefanovich and Bogdan Lazoryak	Crystal structure of new phosphates Ca <sub>9-x</sub> Pb <sub>x</sub> Eu(PO <sub>4</sub> ) <sub>7</sub> from Rietveld refinement	S101
Jacek Podwórny	Temperature dependence of the inversion degree in three-cation spinel solid solutions: experimental evaluation by XRD	S104
Kristian Ufer, Reinhard Kleeberg and Thomas Monecke	Quantification of stacking disordered Si–Al layer silicates by the Rietveld method: application to exploration for high-sulphidation epithermal gold deposits	S111

Stefano Checchia,  
Marco Scavini, Mattia Allieta,  
Michela Brunelli,  
Claudio Ferrero and  
Mauro Coduri

Size and spatial correlation of defective domains in yttrium-doped CeO<sub>2</sub>

S119

Simone T. B. de Salvi, Diego  
Luiz Tita, Carlos de O. Paiva-  
Santos and Selma G. Antonio

Characterization of hydrochlorothiazide in solid formulations

S127

## **ERRATUM**

*Powder Diffraction* Volume 28 / Supplement 2 / September 2013– ERRATUM

S131

# 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 Nanshanjie, 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 Nanshanjie, Zhongguancun, Haidian District,  
Beijing 100190,  
China  
gangwang@iphy.ac.cn

On the Cover: **Top-left and bottom-right:** 2D diffraction images collected on a ZnO sample with direct beam in the center of the CCD camera, and on a glass sample with direct beam in the corner of the CCD camera, respectively, at the ID11 beamline of the ESRF. (Courtesy of Andrea Bernasconi, et al. "Total Scattering Experiments on glass and crystalline materials at the ESRF on the ID11 Beamline", these Proceedings). **Top-right:** *in situ*

dehydrogenation and hydrogenation of  $\text{MgH}_2\text{-V}_2\text{O}_5$ . (Courtesy of Dmytro Korablov et al. "Mechanism and kinetics of early transition metal hydrides, oxides and chlorides to enhance hydrogen release and uptake properties of  $\text{MgH}_2$ ", these Proceedings). **Bottom-left:** GISAXS patterns of 40 nm thick films - block copolymers with nanoparticles - together with corresponding AFT phase contrast pattern (Courtesy of J. Dieter et al., "Thin film morphologies of block copolymers with nanoparticles", these Proceedings).

*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@mrsvica.com](mailto:mjmrvica@mrsvica.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 form 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)