Powder Diffraction

	Editorial	1
D. B. Sullenger, J. S. Cantrell, and T. A. Beiter	X-ray powder diffraction patterns of energetic materials	2
M. Dolores Marcos, Pedro Amorós, Daniel Beltrán, and Aurelio Beltrán	X-ray powder diffraction data for some transition metal phosphites and hypophosphites	15
A. R. Ginting, B. H. O'Connor, and J. G. Dunn	X-ray powder data for synthetic dolerophanite, $copper(II)$ oxysulphate $[Cu_2O(SO_4)]$	21
D. P. Matheis, R. L. Snyder	X-ray powder diffraction analysis of the incommensurate modulated structure of $Bi_2Sr_2CaCu_2O_8$	28
Sampath S. Iyengar	High-temperature X-ray powder diffraction analysis of selected ceramic mixtures	38
Richard A. Vaia, Maura S. Weathers, and William A. Bassett	Anomalous peaks in grazing incidence thin film X-ray diffraction	44
Benjamin L. Ballard, Paul K. Predecki, and Camden R. Hubbard	Residual stresses in a SiC whisker-reinforced alumina composite by high-temperature X-ray diffraction	50
M. Touboul, E. Bétourné, and B. Gérand	New X-ray powder diffraction data for lithium tetrahydroxoborate LiB(OH) ₄	54
C. G. Lindsay, C. J. Rawn, and R. S. Roth	Powder X-ray diffraction data for $Ba_4ZnTi_{11}O_{27}$ and $Ba_2ZnTi_5O_{13}$	56
G. Artioli, M. Bellotto, and B. Palosz	High-temperature in situ Rietveld study of Fe,Mg cation partitioning in olivine	63
Paolo Ballirano, Adriana Maras, Peter R. Buseck, Su Wang, and Ann M. Yates	Improved powder X-ray data for cancrinites I: Afghanite	68
	International Report	74
	Calendar of Meetings	74
	Meeting Reports	76
	Book Reviews	78
	Computer Comments	80
	Cumulative Author Index	82



Volume 9 Number 1 March 1994

https://doi.org/10.1017/Powder9Diffractiony CambriAnninternational journal of materials characterization

SIEMENS

X-ray Vision

Wouldn't it be nice to have X-ray vision to analyze your samples?

It's possible with GADDS^{**}, the General Area Detector Diffraction System from Siemens. GADDS provides fast and simple X-ray analysis of powders, polymers, thin films, and coatings.

Recent innovations in hardware and software from Siemens make X-ray technology a practical tool for your applied chemistry, process control, or research and development needs.

Applications include texture analysis, small angle scattering, and detailed qualitative and quantitative molecular level measurements.

Depending upon your needs, a system can be configured to perform a wide variety of analyses — all requiring just minutes of inspection time.



To learn more about the analytical X-ray instrumentation from Siemens, call 1-800-234-XRAY.



© 1994 Siemens Analytical Instrumentation



See us at pittCON booth #5429



In USA and Canada contact: Siemens Analytical Instrumentation Division, 6300 Enterprise Lane, Madison, WI 53719 (800) 234-XRAY FAX: (608) 276-3006. Worldwide contact: Siemens AG, Analytical Systems, AUT V371, D76181 Karlsruhe 21, Germany (0721) 545-4295 FAX: (0721) 595-4506.

The Third Edition of the SPEX Handbook answers questions about Producing homogeneous powders Making pressed or fused pellets Controlling contamination Eliminating particle size effects Handling liquid samples Selecting and ordering products

The SPEX Handbook includes:

Open-Vessel Microwave Digestion System

> Automated 35-ton Hydraulic X-Press

Automated SPEX-Claisse Fusion Fluxers

Cryogenic Laboratory Mill Graphite Crucibles For Fusion XRF Liquid Cells and Window Films Boron Carbide Mortars and Pestles Manual and Motorized Laboratory Presses Evacuable Pellet Dies and Spec-Caps Graphite Crucibles for Fusions D Nylon Sieve Sets Shatterboxes, Mixer/Mills . . . AND MORE!

SPEX INDUSTRIES, INC. 3880 PARK AVE • EDISON, N.J. 08820 TEL: 908-549-7144 • FAX: 908-503-9647

See us at GCC, ALEX, FACSS and GSA.

2635

CONTRACTOR OF THE STATE



Powder Diffraction

An International Journal of Materials Characterization

Editor in Chief

Deane K. Smith Department of Geosciences The Pennsylvania State University 239 Deike Building University Park, PA 16802-2711U.S.A.

Managing Editor

Ron Jenkins JCPDS-International Centre for Diffraction Data 12 Campus Blvd., Newtown Square, PA 19073-3273 U.S.A.

Editor for New Diffraction Data

Gregory J. McCarthy Department of Chemistry North Dakota State University Fargo, ND 58105-5516 U.S.A.

European Editor

Jan W. Visser Henry Dunantlaan 81, 2614 GL Delft, Netherlands

Editor for Australia and New Zealand

Brian H. O'Connor Curtin University GPO Box U 1987, Perth 6001 Western Australia, Australia

Editor for Japan

Hideo Torava **Ceramics Research Lab** Nagoya Institute of Technology Asahigaoka, Tajima 507 Japan

International Reports Editor

Helein D. Hitchcock NASA DM-MSL-1 Kennedy Space Center, FL 32899 U.S.A.

Assistant to the Managing Editor Mary M. Rossi

Editorial Advisory Board

C. S. Barrett, Denver, Colorado P. Bayliss, Sydney, Australia

- C. Z. Bojarski, Katowice, Poland
- A. Brown, England
- D. Cox, Upton, New York
- W. Eysel, Heidelberg, West Germany J. Fiala, Plzeň, Czech Republic
- V. A. Frank-Kamenetsky, Leningrad, U.S.S.R.
- L. Frevel, Midland, Michigan
- P. Gado, Budapest, Hungary
- H. Goebel, Munchen, West Germany
- T. Huang, San Jose, CA (IUCr Representative)
- G. G. Johnson Jr., State College, Pennsylvania Q. Johnson, Livermore, California
- J. I. Langford, Birmingham, U.K.
- D. Louër, Rennes, France
- H. F. McMurdie, Gaithersburg, Maryland
- M. E. Mrose, Gaithersburg, Maryland
- M. H. Mueller, Argonne, Illinois
- M. Nichols, Livermore, California
- B. Post, Brookline, Massachusetts
- R. L. Snyder, Alfred, New York
- S. Weissmann, Metuchen, New Jersev
- T. Yamanaka, Tokyo, Japan
- R. A. Young, Atlanta, Georgia

AIP Production: Lin Miller, Editorial Supervisor: Andrea Witt, Journal Coordinator; Connie Nedohon, Senior Production Editor

Powder Diffraction is a guarterly journal published for the JCPDS-International Centre for Diffraction Data by the American Institute of Physics (AIP). Powder Diffraction is a journal of practical technique, publishing articles relating to the widest range of application-from mineral 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 (3 copies) to the most appropriate Powder Diffraction Editor listed on this page. The Editors will consider all manuscripts received, but assume no responsibility regarding them. Materials will be returned only when accompanied by appropriate postage. There is no publication charge. See Powder Diffraction Notes for Authors for additional information.

Proofs and all correspondence concerning papers in the process of publication should be addressed to: Editorial Supervisor, Powder Diffraction, AIP, 500 Sunnyside Blvd., Woodbury, NY 11797-2999.

For advertising rates and schedules contact AIP Advertising Department. Orders, advertising copy, and offset negatives should be sent to: Advertising Department, American Institute of Physics, 500 Sunnyside Blvd., Woodbury, NY 11797-2999; phone: (516) 576-2440; fax: (516) 576-2481.

Subscription Prices (1994)

Mexico, Central Europe, Mid-East Asia & U.S.A & Canada & South America & Africa* Oceania* \$75 Individual \$55 \$75 \$75 Institutional or Library \$95 \$95 \$95 \$95

*Subscription rates to Eastern Hemisphere include air freight service.

Back-Number Prices. 1994 single copies: \$30. Prior to 1993 single copies: \$30.

Subscription, renewals, and address changes should be addressed to AIP Circulation and Fulfillment Division (CFD), 500 Sunnyside Blvd., Woodbury, NY 11797-2999. 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 and Back Volumes: 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 AIP Circulation and Fulfillment Division (CFD) at (516) 576-2288; (800) 344-6901. Institutional or library subscribers please contact AIP Subscriber Services at (516) 576-2270; (800) 344-6902

Reprint Billing: Contact: AIP, 500 Sunnyside Blvd., Woodbury, NY 11797-2999, Attn: Reprint Billing; (516) 576-2234; (800) 576-6909.

Copyright Notice: Authorization to photocopy items for internal or personal use, or the internal or personal use of specific clients, is granted by AIP, provided that the appropriate fee per page is paid directly to the Copyright Clearance Center (CCC), 27 Congress Street, Salem, MA 01970.

The item-fee code for this publication is 0885-7156/94 \$6.00.

Permission For Other Use: Individual teachers, students, researchers, and libraries acting for them are permitted to make copies of articles in this journal for their own use in research or teaching, including multiple copies for classroom or library reserve use, provided such copies are not sold. Copying for sale is subject to payment of copying fees. Permission is granted to quote from the journal with the customary acknowledgment of the source. To reprint a figure, table, or other excerpt requires in addition the consent of one of the original authors and notification to AIP. Reproduction for advertising or promotional purposes, or republication in any form, is permitted only under license from AIP, which will normally require that the permission of one of the authors also be obtained. Direct inquiries to: AIP Office of Rights and Permissions, 500 Sunnyside Blvd., Woodbury, NY 11797-2999.

Document Delivery: Copies of individual articles may be obtained at \$15 per article for Institutions and \$12 per article for Individuals (postage included). Airmail and fax service are also available. Contact: AIP Circulation and Fulfillment (CAF) Division, 500 Sunnyside Blvd., Woodbury, NY 11797-2999; phone: (516) 576-2277; (800) 344-6908; fax: (516) 394-9704; E-mail; elecpub@pinet.aip.org.

Powder Diffraction (ISSN: 0885-7156) is published quarterly (4X annually) by the American Institute of Physics for the JCPDS-International Centre for Diffraction Data, 500 Sunnyside Blvd., Woodbury, NY 11797-2999. JCPDS-ICDD principal office: 12 Campus Blvd., Newtown Square, PA 19073-3273. POSTMASTER: Send address changes to Powder Diffraction, American Institute of Physics, 500 Sunnyside Blvd., Woodbury, NY 11797-2999. Second class postage rates paid at Woodbury, NY and additional mailing offices

Copyright 1994 by JCPDS-International Centre for Diffraction Data

Expand your x-ray diffraction capabilities not your overhead.

Whether you just need services or your XRD lab is on "overload," IC Laboratories provides every testing service and advanced capability you need in qualitative or quantitative x-ray diffraction analysis — from austenite to zeolites, from air filters to thin films. You are assured of rapid turn-around of results — as little as 48 hours — because IC Labs is one of the most highly automated commercial labs in the U.S., with knowledgeable personnel ready to address all your applications. For a copy of our technical prospectus, contact IC Laboratories.

IC Laboratories

Post Office Box 721 Amawalk, New York 10501 (914) 962-2477

entre for Diffra

We're the Specialists in XRD

ICDD Clinics on X-ray Powder Diffraction and X-ray Fluorescence Spectrometry

Fundamentals of X-ray Powder Diffraction June 6–10, 1994

Covering theoretical discussion of instrumentation (both diffractometer and camera methods), specimen preparation, data acquisition, and qualitative phase analysis.

Advanced Methods in X-ray Powder Diffraction June 13–17, 1994

Emphasizing computer-based methods of data collection and interpretation, both for qualitative and quantitative phase analysis.

Fundamentals of X-ray Fluorescence June 20–24, 1994

Covering basics of X-ray spectra, instrumentation design, methods of qualitative and quantitative analysis, specimen preparation and applications for both wavelength and energy dispersive spectrometry.

Advanced Methods in X-ray Fluorescence

June 27–July 1, 1994

Emphasizing quantitative methods, use of automated Xray spectrometers, review of mathematical matrix correction procedures, and new developments in XRF.

For further information contact: Theresa Maguire 12 Campus Boulevard, Newtown Square, Pennsylvania, 19073-3273, U.S.A. Phone (610) 325-9814, FAX (610) 325-9823

International Centre for Diffraction Data

Diffraction Reference Standards and Zero-background Sample Plates Custom Designed and Built for any Application Your first step to improved x-ray diffraction results should be to ontact The Gem Dugout for quality diffraction alignment standards and And the next step is successful zero-background plates. ray diffraction results. Gem Dugout 52 Princeton Drive ate College, PA 16803 865-5 14)

INDEX TO ADVERTISERS

Dapple Systems	A2
Gem Dugout	A5
ICDD	A4, A5, A6
IC Labs	A4
McCrone Scientific Ltd	A5
Scintag, Inc	Cover 4
Seifert X-Ray Corp	Cover 3
Siemens Analytical	Cover 2
SPEX	A1

Advertising Sales Office

American Institute of Physics 500 Sunnyside Boulevard Woodbury, N.Y. 11797-2999 Telephone: (516) 576-2440 Advertising Fax: (516) 576-2481

Advertising Director Edward P. Greeley Advertising Manager Richard T. Kobel

Asst. Advertising Manager Advertising Representative Arnie W. Schweitzer Robert G. Finnegan

> Production Wendy Cona

McCRONE MICRONISING MILL

- Reproducible mean particle size for XRD and IR
- Rapid, unique grinding action (not a ball mill)
- Wet grinding minimises damage to sample crystallinity
- Choice of grinding elements (agate or corundum)
- World McCrone Scientific Limited, 73 Maygrove Road, London NW6 2BP UK. Tel: 071 624 5409 Fax: 071 372 4415
- USA McCrone Accessories and Components 850 Pasquinelli Drive, Westmont Illinois 60559. Tel: 708 887 7100 Fax: 708 887 7764

For 1993/94 from ICDD...



EDD^{Electron Diffraction} Data Base

(NIST/Sandia/ICDD) Crystallographic & chemical data on over 81,000 crystalline materials.†



IST Crystal Data File

Crystallographic & chemical data on over 182,500 crystalline materials.*

†Available for IBM-PC compatibles, VAX & Macintosh *Available for IBM-PC compatibles & VAX

International Centre for Diffraction Data 12 Campus Blvd., Newtown Square, PA 19073-3273, U.S.A. Phone: 215/325-9810; FAX: 215/325-9823





Your source for X-ray Diffraction Data

The Powder Diffraction File—

Over 58,000 patterns

PC-PDF —

A unique scientific database

PC-PDF, a high density, data storage/retrieval system, uses a personal computer equipped with a CD-ROM drive and disk which contains the entire PDF-2 database and index files.

Speed and flexibility

PC-PDF, through use of optimum packing and access algorithms, displays results within seconds. You can, for example:



Other Files, Publications & Services

- On CD-ROM: NIST Crystal Data File
- On magnetic tape or floppy disks:
- Electron Diffraction Database
- In print:

Metals and Alloys Indexes – a 680-page book containing Alphabetical Index Pearson Symbol Code Index Common Names Index Strukturbericht Symbol Index Minerals Databooks... Search Manuals... Educational Materials...

Powder Diffraction, a quarterly journal

• Regularly scheduled clinics, workshops and short courses.

For information contact —

M. M. Fornoff Sales/Marketing Manager International Centre for Diffraction Data 12 Campus Boulevard Newtown Square Pennsylvania 19073-3273, U.S.A. FAX 215/325-9823

