



# Powder Diffraction

An international journal of materials characterization

Volume 12 Number 3 September 1997

33-1161  
SiO<sub>2</sub>  
Silicon Oxide  
Quartz, syn

Rad. CuKα, λ 1.540598 Filter Mono. d-sp Diff.  
Cut off Int. Diffractometer I/I<sub>0</sub> 3.6  
Ref. Natl. Bur. Stand. (U.S.) Monogr. 25, 18 61 (1981)

Sys. Hexagonal  
a 4.9133(2) b  
c 5.4053(4) α  
β  
γ  
D<sub>5</sub> 2.65 D<sub>6</sub> 2.66  
Ref. Swanson, Fuyat, Natl. Bur. Stand. (U.S.), Circ. 539, 3 24 (1954)

Colorless  
Pattern taken at 25°C. Sample from the Glass Section at NBS, Gaithersburg, Maryland, USA. Reviewed by Holzer, University, Fargo, North Dakota, USA. Agrees well with experimental Quartz group. Also called: silica as internal standard. PSC: hP9. Calculated pattern. Plus 6 additional reflections to 0.9089.

S.G. P3,21 (154)  
A Z 3 mp C 1.1001  
SS/FOM F<sub>0</sub>=77(013,31)  
ey 1.553 Sign + 2V  
Ref. Stand. (U.S.), Circ. 539, 3 24 (1954)

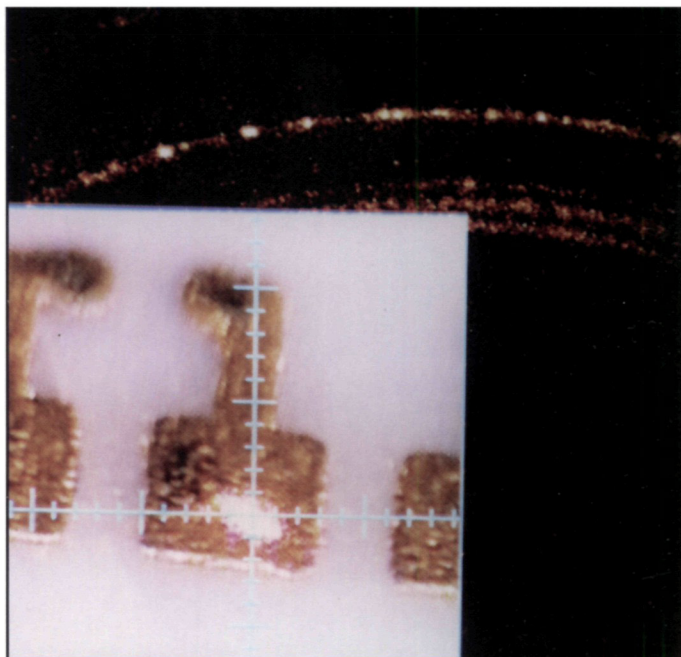
| dÅ     | Int | hkl | dÅ     | Int | hkl |
|--------|-----|-----|--------|-----|-----|
| 4.257  | 22  | 100 | 1.1532 | 1   | 311 |
| 3.342  | 100 | 101 | 1.1405 | <1  | 204 |
| 2.457  | 8   | 110 | 1.1143 | <1  | 303 |
| 2.282  | 8   | 102 | 1.0813 | 2   | 312 |
| 2.237  | 4   | 111 | 1.0635 | <1  | 400 |
| 2.127  | 6   | 200 | 1.0476 | 1   | 105 |
| 1.9792 | 4   | 201 | 1.0438 | <1  | 401 |
| 1.8179 | 14  | 112 | 1.0347 | <1  | 214 |
| 1.8021 | <1  | 003 | 1.0150 | <1  | 223 |
| 1.6719 | 4   | 202 | 0.9898 | 1   | 402 |
| 1.6591 | 2   | 103 | 0.9873 | 1   | 313 |
| 1.6082 | <1  | 210 | 0.9783 | <1  | 304 |
| 1.5418 | 9   | 211 | 0.9762 | 1   | 320 |
| 1.4536 | 1   | 113 | 0.9636 | <1  | 205 |
| 1.4189 | <1  | 300 |        |     |     |
| 1.3820 | 6   | 212 |        |     |     |
| 1.3752 | 7   | 203 |        |     |     |
| 1.3718 | 8   | 301 |        |     |     |
| 1.2880 | 2   | 104 |        |     |     |
| 1.2558 | 2   | 302 |        |     |     |
| 1.2285 | 1   | 220 |        |     |     |
| 1.1999 | 2   | 213 |        |     |     |
| 1.1978 | 1   | 221 |        |     |     |
| 1.1843 | 3   | 113 |        |     |     |
| 1.1804 | 3   | 313 |        |     |     |



# SIEMENS

## *X-ray Diffraction for Microanalysis*

**Powerful  
Flexible  
Rapid**



Siemens' General Area Detector Diffraction System (GADDS) with the HI-STAR area detector provides you with a more powerful, flexible, and faster microanalysis solution than any other commercially available system. Combined laser and video sample alignment provides real-time color displays of both the diffraction pattern and the region under investigation (as shown with the microchip sample above). These regions can be selected manually with "point-and-shoot" capabilities or in predefined arrays, permitting Diffraction Function Mapping (DFM) studies. Using an optional crossed Göbel Mirror system with a GADDS can also provide increased X-ray flux, eliminating the need for a rotating anode X-ray source.

- Ideal for studying very small samples or microdefects on large samples
- Rapid data collection with HI-STAR, Siemens' unique 2-dimensional detector technology
- Suitable for investigating plastics, metals, ceramics, geological and forensic samples, semiconductors, superconductors, and many other materials
- Measures scattering from amorphous, polycrystalline, and single-crystal materials

**For More information on  
Siemens' X-ray Diffraction  
Systems, contact Siemens  
Analytical X-ray Systems at:**

**800-234-XRAY**

(In the U.S.A. and Canada)

Direct Dial: 608-276-3000

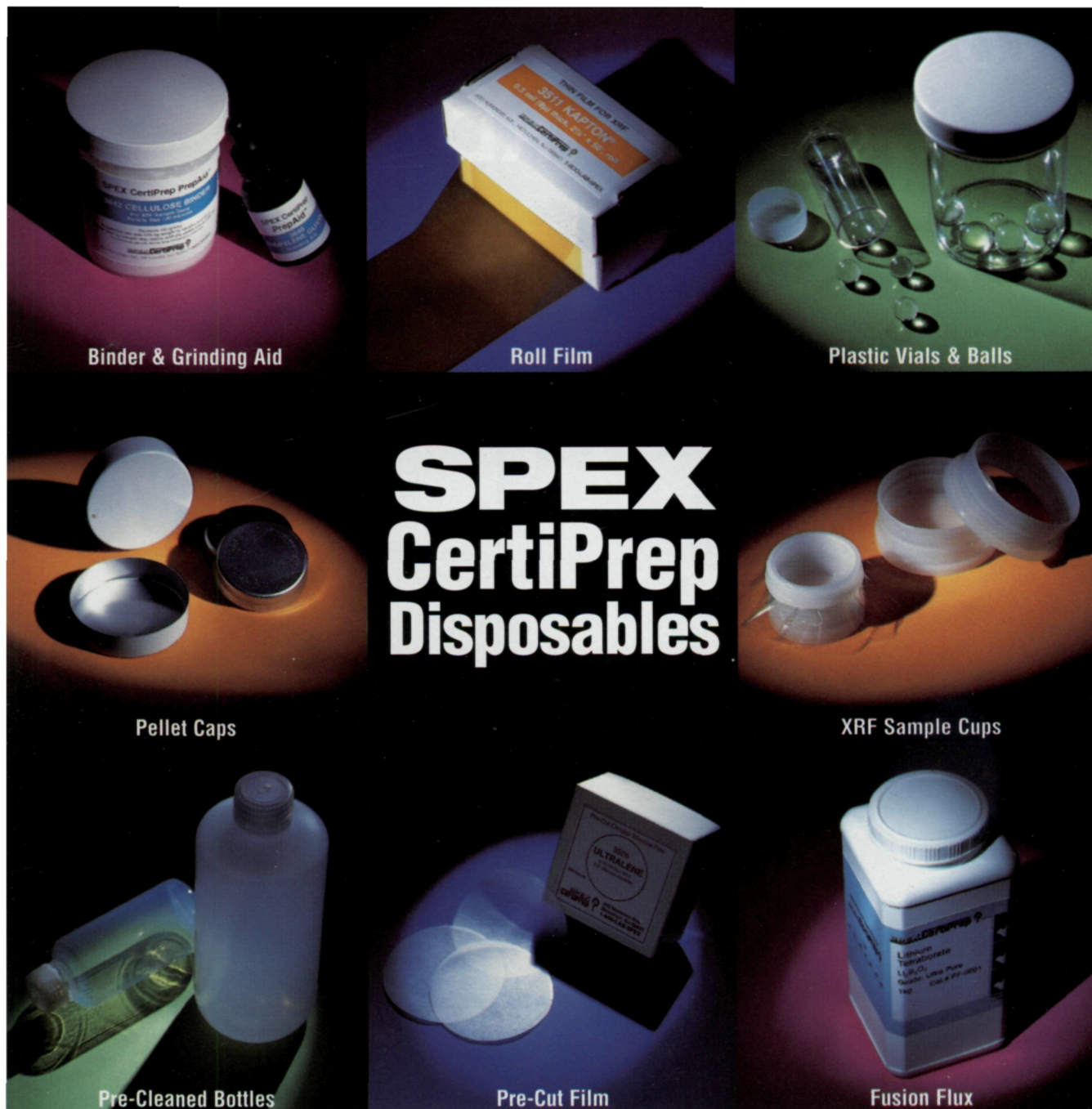
Fax: 608-276-3006

Email: [info@siemens-xray.com](mailto:info@siemens-xray.com)

Internet Homepage: <http://www.siemens-xray.com>

In North America contact: **Siemens Analytical X-ray Systems, Inc.**, 6300 Enterprise Lane, Madison, WI 53719-1173 USA  
Outside North America contact: **axs Analytical X-ray Systems GmbH**, D-76181 Karlsruhe, Germany, Phone: +49-721-595-2888, Fax: +49-721-595-4587

# The Most Important Materials In XRF Spectroscopy...Next To Your Samples



Binder & Grinding Aid

Roll Film

Plastic Vials & Balls

Pellet Caps

XRF Sample Cups

Pre-Cleaned Bottles

Pre-Cut Film

Fusion Flux

## SPEX CertiPrep Disposables

For accurate and uniform analytical results, you need reliable and consistent sample preparation. SPEX CertiPrep has been supplying XRF spectroscopists with quality sample preparation and handling products for over forty years.

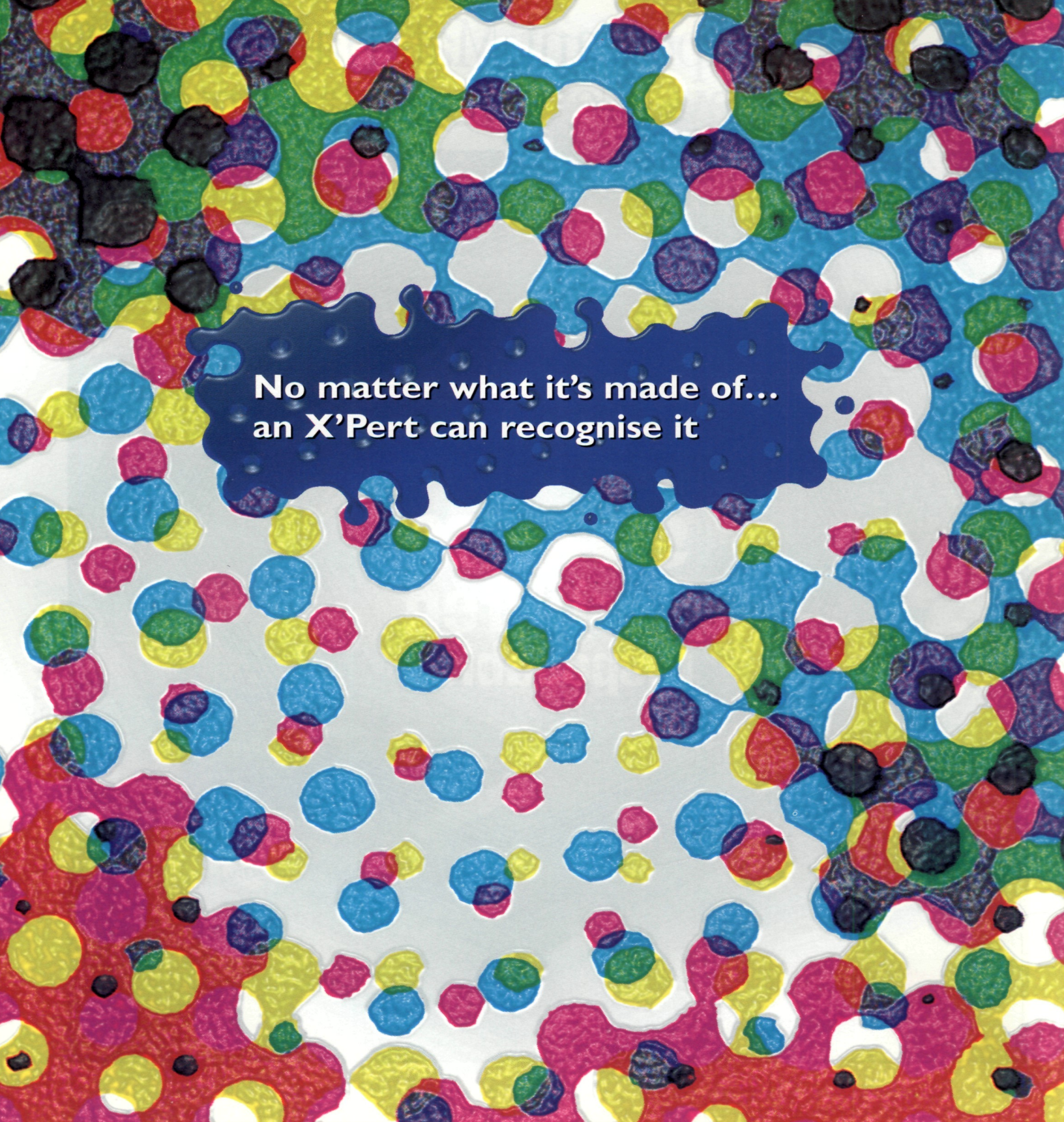
Whether you press powders in dies or fuse them into glass discs, or if you use sample cells to run liquids, powders, pastes, or other materials, we have the supplies and equipment to get the job done. We can help you choose the proper binder, grinding aid, or borate flux for your particular sample. SPEX CertiPrep also provides the most complete line of mills, presses, dies, and fusion fluxers.

Our commitment to Total Customer Satisfaction means: "Serving our customers promptly and courteously, with unsurpassed technical and

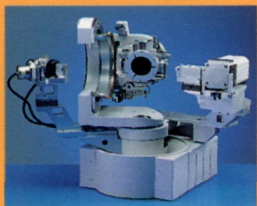
applications support, and top quality, reliable SPEX CertiPrep products." Call, FAX, or e-mail for your copy of our catalog, *The Handbook of Sample Preparation and Handling*. **1 800 LAB-SPEX**

**SPEX  
CertiPrep**

203 Norcross Avenue ■ Metuchen, NJ 08840 USA ■ 908-549-7144  
Fax 908-603-9647 ■ SamplePrep@spexcsp.com ■ <http://www.spexcsp.com>



No matter what it's made of...  
an X'Pert can recognise it



**PHILIPS X'PERT  
MRD SYSTEMS**

With the Philips X'Pert x-ray diffractometer line, you'll find a solution to even the most complex materials identification problems. X'Pert-MRD for advanced research, X'Pert MPD for powder diffraction, stress/texture, microstructure and crystallographic studies. A comprehensive hardware/software range offering unique features for ultimate accuracy, sensitivity, flexibility and ease of use.

Netherlands: +31 (546) 83 94 30 or fax +31 (546) 89 35 98

E-Mail: [Pieter.deGroot@nl.cis.philips.com](mailto:Pieter.deGroot@nl.cis.philips.com)

Internet: <http://www.philips.com/axr>

*Let's make things better.*



**PHILIPS**

## An International Journal of Materials Characterization

### Editor-in-Chief

Deane K. Smith  
1652 Princeton Drive  
State College, PA 16803-3257 U.S.A.

### Associate Editor-in-Chief

Ting C. Huang  
6584 Radko Drive  
San Jose, CA 95119-1924 U.S.A.

### Managing Editor

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

### Editor for New Diffraction Data

Ting C. Huang  
6584 Radko Drive  
San Jose, CA 95119-1924

### 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 Toraya  
Ceramics Research Lab  
Nagoya Institute of Technology  
Asahigaoka, Tajima 507 Japan

### International Reports Editor

Ting C. Huang

### Editorial Advisory Board

P. Bayliss, Sydney, Australia  
C. Z. Bojarski, Katowice, Poland  
A. Brown, Dorset, England  
D. Cox, Upton, New York  
W. Eysel, Heidelberg, Germany  
J. Fiala, Pízeň, Czech Republic  
L. Frevel, Midland, Michigan  
P. Gado, Budapest, Hungary  
H. Goebel, Munchen, Germany  
R. Jenkins, Newtown Square, Pennsylvania  
G. G. Johnson Jr., State College, Pennsylvania  
Q. Johnson, Livermore, California  
J. I. Langford, Birmingham, U.K.  
D. Louër, Rennes, France  
G. J. McCarthy, Fargo, North Dakota  
H. F. McMurdie, Gaithersburg, Maryland  
M. E. Mrose, Gaithersburg, Maryland  
M. Nichols, Livermore, California  
R. L. Snyder, Columbus, Ohio  
E. K. Vasil'ev, Irkutsk, Russia  
T. Yamanaka, Tokyo, Japan  
R. A. Young, Atlanta, Georgia

**AIP Production:** Lin Miller, Editorial Supervisor  
Andrea Witt, Journal Coordinator  
Kelly Quigley, Senior Production Editor

**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.

*Powder Diffraction* is a quarterly 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 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.

**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 (1997)

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

\*Subscription rates to Eastern Hemisphere include air freight service.

**Back-Number Prices.** 1997 single copies: \$30. Prior to 1997 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 Circulation and Fulfillment Division, Woodbury, NY 11797-2999; (516) 576-2234; (800) 344-6909.

**Copying:** Single copies of individual articles may be made for private use or research. Authorization is given (as indicated by the Item Fee Code for this publication) to copy articles beyond the use permitted by Sections 107 and 108 of the U.S. Copyright Law, provided the copying fee of \$6 per copy per article is paid to the Copyright Clearance Center, 222 Rosewood Drive, Danvers, MA 01923, USA. Persons desiring to photocopy materials for classroom use should contact the CCC Academic Permissions Service. The Item Fee Code for this publication is 0885-7156/96 \$6.00.

Authorization does not extend to systematic or multiple reproduction, to copying for promotional purposes, to electronic storage or distribution, or to republication in any form. In all such cases, specific written permission from AIP must be obtained.

**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 AIP.

**Requests for Permission:** Address requests to AIP Office of Rights and Permissions, 500 Sunnyside Boulevard, Woodbury, NY 11797-2999; Fax: 516-576-2327; Telephone: 516-576-2268; Internet: rights@aip.org.

**Document Delivery:** Copies of articles can be ordered for \$15 per copy from the AIP/Member Society document delivery service, "Articles in Physics," 75 Varick Street, New York, NY 10013; Fax: 212-301-4060; Telephone: 800-480-PHYS (800-480-7497) (in U.S. and Canada), or 212-301-4000; E-mail: articles@aip.org; URL: <http://www.aip.org/articles.html>.

**Reprints:** Reprints can be ordered with or without covers only in multiples of 50 (with a minimum of 100 in each category) from AIP, Circulation & Fulfillment/Reprints, 500 Sunnyside Boulevard, Woodbury, NY 11797-2999; Fax: 516-349-9704; Telephone: 800-344-6909 (in U.S. and Canada), or 516-576-2234.

*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. Periodicals postage paid at Woodbury, NY and additional mailing offices.

**Online Availability:** Abstracts of journal articles published by the AIP and Member Societies (and several other physics publishers) are available in the SPIN database via the AIP online service PINET. Also available on PINET are *Advance Abstracts*, a current awareness service, other physics information resources, as well as internet services (Internet: elecprod@aip.org).

**Copyright © 1997 by JCPDS-International Centre for Diffraction Data. All rights reserved.**



**Rigaku**

PUTTING X-RAYS TO WORK THE WORLD OVER



# Plug 'N Play XRD

Put Rigaku's Miniflex+ to Work for You.

- › Rigaku's Plug 'N Play XRD System is the solution for your chemical and phase analysis needs. This new, low-cost Table-top X-ray Diffractometer expands general laboratory capabilities by making X-ray diffraction easily accessible to everyone.
- › Use Rigaku's Miniflex+ for diffraction pattern "fingerprinting" of your materials. Let Rigaku's XRD Systems identify and quantify your crystalline compounds and structures.
- › This high performer is fast, portable, easy to use, and is non-destructive to the sample. Rigaku's fully automated Plug 'N Play XRD System, the Miniflex+ opens up new applications in QA/QC and is also ideal as an educational tool.

**Rigaku**

*Keeping You at the Forefront  
of Your Technology*

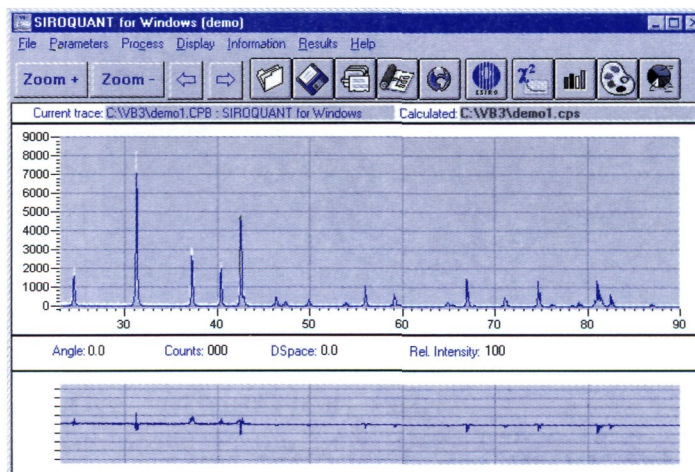
|                                                                           |                                                                                                                                                              |     |
|---------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|
| Deane K. Smith                                                            | Editorial: Donating Used X-ray Equipment to ICDD                                                                                                             | 133 |
| Liangqin Nong, Lingmin Zeng, and Jianmin Hao                              | X-ray powder diffraction data for compound DyNiSn                                                                                                            | 134 |
| Zong-ming Jin, Zheng Jin, and Fang Huang                                  | X-ray powder diffraction analysis of an organic material for nonlinear optics 3-methyl-4-methoxy-4'-nitrostilbene                                            | 136 |
| C. Colbeau-Justin, G. Wallez, A. Elfakir, and M. Quarton                  | Revised crystallographic data of $K_2MgGeO_4$ and $K_2CdGeO_4$ compounds                                                                                     | 138 |
| D. Y. Li, C. W. MacKinnon                                                 | Indexing of incommensurate satellite reflections in X-ray powder diffraction pattern of $(Bi, Pb)_2Sr_2Ca_2Cu_3O_x$ (2223) phase                             | 141 |
| Chi-Tang Li                                                               | Development of a simple device for a moisture-proof X-ray diffraction analysis                                                                               | 145 |
| Vicente Esteve, Juan Carda, María Mercedes Reventós, and José María Amigó | Quantitative X-ray diffraction phase analysis of airborne particulate collected by a cascade impactor sampler using the Rietveld full-pattern fitting method | 151 |
| E. Bétourné, M. Touboul                                                   | Crystallographic data about hydrated and anhydrous lithium monoborates                                                                                       | 155 |
| P. Riello, P. Canton, and G. Fagherazzi                                   | Calibration of the monochromator bandpass function for the X-ray Rietveld analysis                                                                           | 160 |
| D. D. Nihtianova, I. T. Ivanov, J. J. Macicek, and I. K. Georgieva        | Crystallographic data for $BaMnSiO_4$ : A new phase in the system BaO-MnO-SiO <sub>2</sub>                                                                   | 167 |
| M. Lucco-Borlera, D. Mazza, L. Montanaro, A. Negro, and S. Ronchetti      | X-ray characterization of the new nasicon compositions $Na_3Zr_{2-x}Si_{2-x}P_{1+x}O_{12}$ with $x = 0.333, 0.667, 1.000, 1.333, 1.667$                      | 171 |
| K. D. Rogers                                                              | Initial Rietveld characterisation of biological calcifications                                                                                               | 175 |
| D. Louër, J. M. Criado, M. J. Dianez, and L. A. Perez-Maqueda             | X-ray powder diffraction study of the thermal behavior of barium titanium citrate hydrate                                                                    | 180 |
|                                                                           | International Report                                                                                                                                         | 185 |
|                                                                           | Calendar of Meetings                                                                                                                                         | 185 |
|                                                                           | Regional Reports                                                                                                                                             | 187 |
|                                                                           | Invited Papers                                                                                                                                               | 187 |
|                                                                           | Poster Session                                                                                                                                               | 189 |
|                                                                           | Short Courses and Workshops                                                                                                                                  | 191 |
|                                                                           | Notes for Author                                                                                                                                             | 193 |
|                                                                           | Cumulative Author Index                                                                                                                                      | 197 |

# SIROQUANT

CSIRO  
AUSTRALIA



Process X-ray Diffractometer  
D5000 matic



## Quantitative XRD

For material investigation and characterisation the **SIEMENS D5000** opens the way to high precision X-ray diffraction in industrial environments.

**SIROQUANT**® is a standardless quantitative XRD phase analysis software package for the Windows™ operating system.

It is suitable for any automated diffractometer.

**SIROQUANT**® was developed to enable quantitative analysis of crystalline phases in rocks, manufactured products, etc. The ever increasing database presently includes over 300 phases.

**SIROQUANT**® provides full-profile Rietveld XRD analysis of all crystalline and poorly crystalline phases.

**Minerals, Cements, Raw Coal & Coal Ash, Metals, Clays, Beach Sands and Inorganic Materials.**

Developed in conjunction with the CSIRO in Australia, **SIROQUANT**® is available directly from **SIETRONICS Pty Limited** or through your local **SIEMENS AG** office.



# Sietronics

Analytical X-ray Systems

Windows™ is a trademark of Microsoft Corporation.  
All trademarks are the properties of their respective owners.

PO Box 3066, Belconnen, ACT, 2617, AUSTRALIA  
Telephone 61.6 251 6611: Facsimile 61.6 251 6659  
Email: [sietron@ibm.net](mailto:sietron@ibm.net)



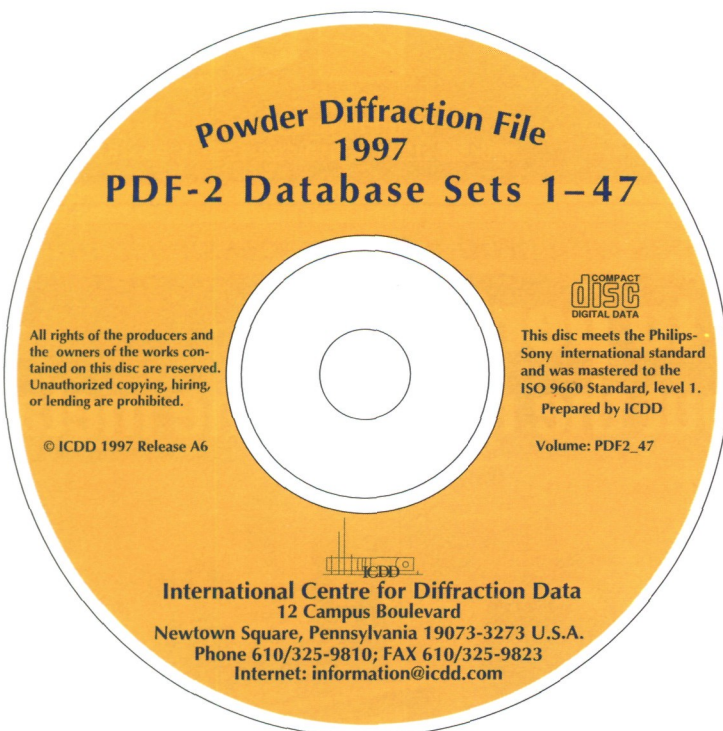


# International Centre for Diffraction Data



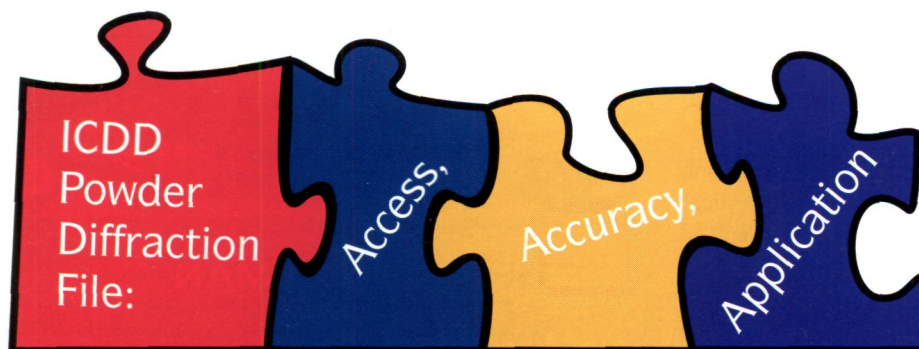
## The Powder Diffraction File

Approximately 66,000 powder diffraction patterns  
in one easy to access database on CD-ROM.



### For information contact:

Dina Tulli  
Assistant to the  
Business Manager-Sales  
12 Campus Boulevard  
Newtown Square  
Pennsylvania 19073-3273  
U.S.A.  
(610) 325-9810  
FAX (610) 325-9823  
Internet: info@icdd.com

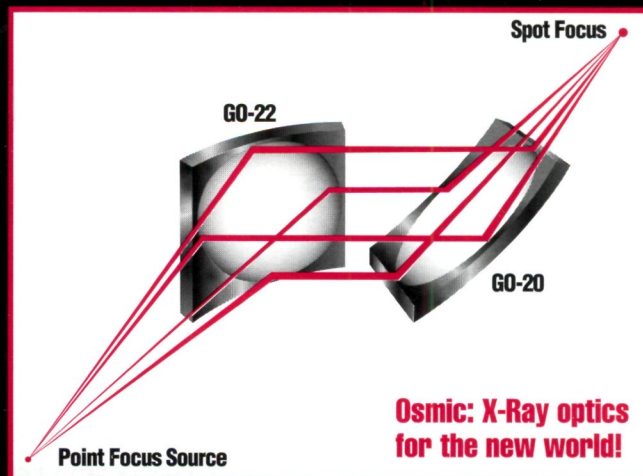


# Gutman Optics™... Transport the Highest Possible x-ray flux to your sample or detector.

Gutman Optics: Osmic's newly created family of curved x-ray mirrors with graded d-spacing multilayer coatings, provide x-ray beams with parallelism better than 0.3 arcmin or focus smaller than 100(μm).

Gutman Optics provide intensity gains of more than an order of magnitude on your sample, and can be successfully applied to diffractometry, microdiffractometry, fluorescent microanalysis, total reflection fluorescent analysis and many other applications.

Call for information on how Osmic can help you apply Gutman Optics.



Osmic: X-Ray optics  
for the new world!



OVONYX™  
Manufacturers of OVONYX™

**Osmic** Inc.  
An Advanced Materials and Technology Company

1788 Northwood Drive ▪ Troy, MI 48084-5532  
800-366-1299 ▪ 810-362-1290 ▪ FAX 810-362-4043

Get specialty beryllium prototypes with production processing in mind.

## Driven to perform? Come to us. We'll put the metal to the metal.

When your production schedule is short, you want to get it done right the first time. You can eliminate a major uncertainty when you entrust your custom beryllium fabrication, joining and coating to us. We'll help you shine.

Here's what we can do for you:

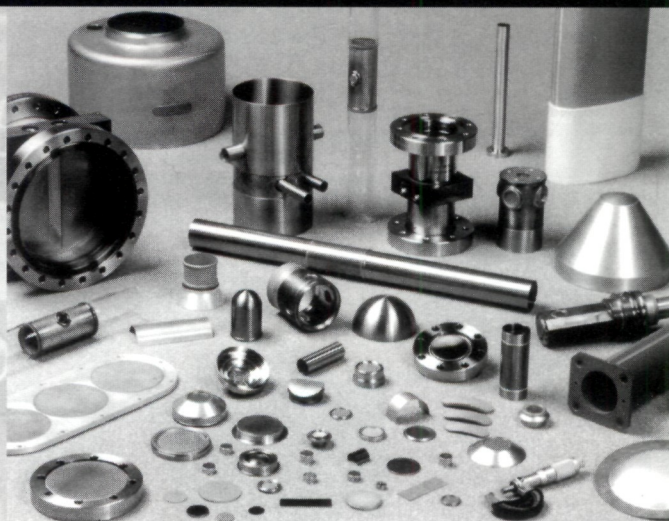
- Depend on us as the only fully integrated source for beryllium sheet and foil products. All critical operations are performed in-house for seamless excellence.
- We're your partner in joining and coating metals. When your project involves joining a metal to a metal, you can count on us.
- Come to us for all your UHV beryllium product needs: x-ray windows, chambers, beam pipes and more.
- Rely on our expert engineering. We like challenges. Taking your design concept into reality would be our pleasure.

Count on us for your tough jobs. Keep in mind that we're the only fully integrated source for beryllium products for the analytical, medical, and scientific industries. Challenge us with your "cutting edge" requirements. We look forward to hearing from you.

TEL: 510-623-1500 • FAX: 510-623-7600

E-Mail: [Electrofusion@BrushWellman.com](mailto:Electrofusion@BrushWellman.com)

44036 South Grimmer Boulevard • Fremont, California 94538 • USA

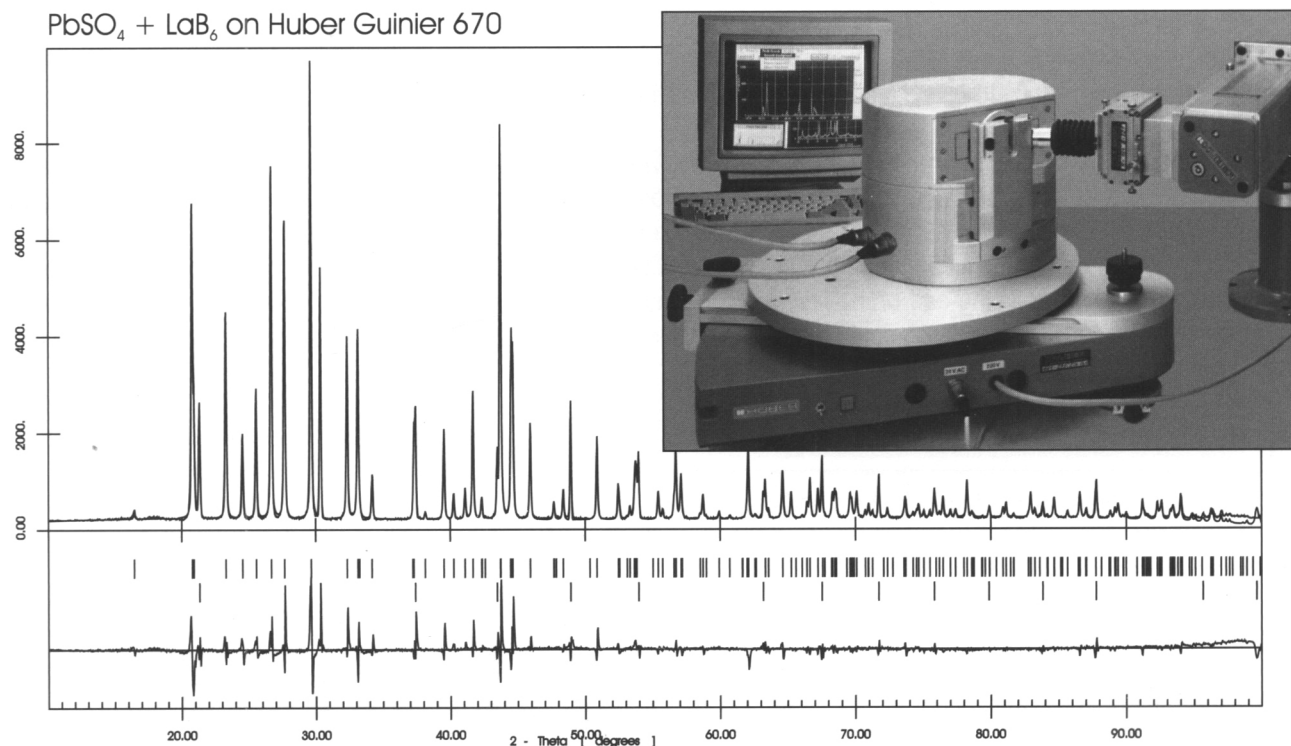


**BRUSHWELLMAN**

ELECTROFUSION PRODUCTS

We're the beryllium window folks.

# *IMAGE PLATE GUINIER CAMERA 670*



### **IMAGE PLATE GUINIER CAMERA 670**

The well established HUBER Guinier Camera 621 has been redesigned to the Model 670 for the use of an image foil instead of the old-fashioned X-ray film. However, it was not only just to fill-in the storage foil into the old film cassette. The whole unit includes the laser scanner and the erasure lamp, as well! This novel instrument combines the high resolution of the X-ray film technique with the extreme fast sensitivity of the image plate detection scheme giving the digital intensity data of the Guinier diffractogram within a couple of minutes, ready for Rietveld-Analysis.

The samples are outside of the closed, and thus evacuable, camera housing.

The Guinier Camera 670 fits onto the Basis 601 and uses any of the Guinier Monochromators of the HUBER Series 611/15. There are options for the flat specimen sample oscillation device 670.1, or for the capillary rotation device 670.2 together with the furnace 670.3 and the high temperature controller 9634. The system includes the data collection and evaluation software running on a PC.

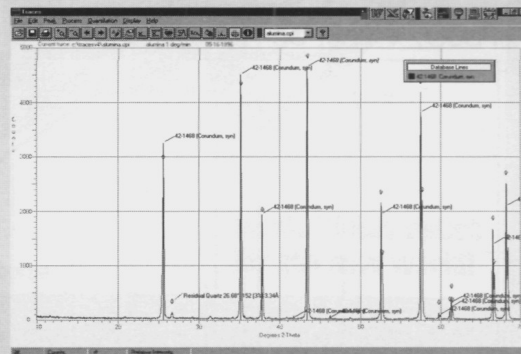
# TRACES Simply The Best!

Advanced XRD Scan Processing for Windows™

TRACESv4 represents the next generation of visual XRD scan processing, providing real operational benefits over the famous TRACESv3. Features like printing PDFcards from your PDF-2, creating your own Mini-database, finding files with a "thumbnail", retrieving database lines by PDF No. Mineral and Chemical name and enhancing your printing of scans with choice of line-styles. DSEARCH is also simply better with AND & OR Chemistry operations, Index files to find phases, better display features and a "Flag" feature to force one-line matches.

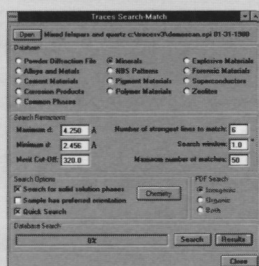
- Σ Integrated Search-Match and peak de-convolution.
- Σ Retained Austenite calculations,
- Indexing and unit cell refinement.
- Σ Manual or automatic peak finding and background removal.
- Σ Report-quality printing on any Windows-compatible printer.

Fast scan display with toolbar and on-line help



- Σ Peak area, FWHM and Scherrer crystallite size.
- Σ Display lines by PDF No., Mineral name, Chemical name.
- Use ICDD or your own Mini Database.
- Σ Subtract, Add, Zero-shift and Trim scans.
- Σ Peak-area based quantitation.
- Batch programming.

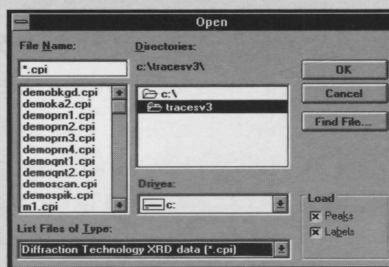
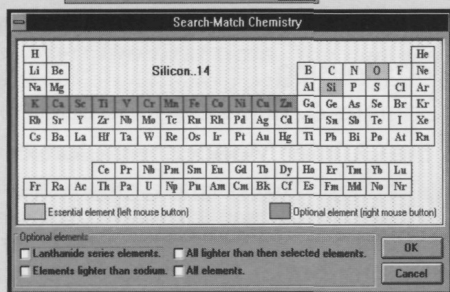
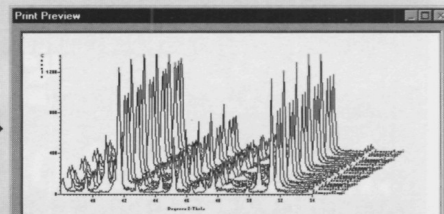
Peak-find to 4 decimal places of 2Theta and 3 decimal places of d-spacing



| Peak Number | 2-Theta Angle | Raw Intensity | d-spacing | Relative Intensity |
|-------------|---------------|---------------|-----------|--------------------|
| 1           | 20.9000       | 145           | 4.250     | 21                 |
| 2           | 21.1000       | 24            | 4.210     | 3                  |
| 3           | 22.0714       | 69            | 4.027     | 10                 |
| 4           | 22.3173       | 37            | 3.983     | 5                  |
| 5           | 22.7400       | 16            | 3.910     | 2                  |
| 6           | 23.0015       | 44            | 3.866     | 6                  |

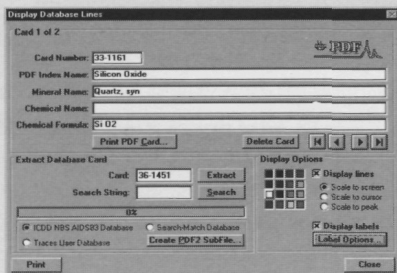
Integrated Search-Match with enhanced functions

Print 100 scans in Isometric or separate, in colour or in monochrome with line-styles and widths of choice.



Process scans from Siemens Philips, Scintag and Rigaku.

Display Database lines, retrieve by all ICDD file header data, print PDF cards, display PDF info on line labels on scan



**Diffraction Technology**

Diffraction Technology Pty. Ltd.  
 Contact : Rod Clapp  
 Phone: 61 6 242 8233  
 FAX: 61 6 242 8266  
 Internet: rod@pcug.org.au  
 www.ozemail.com.au/~difftech/  
 PO Box 444, Mitchell ACT 2911  
 Canberra, Australia.

United States : Jerry Krause  
 Analytical X-ray Instrument Sales  
 Phone/FAX : 303 277 1569

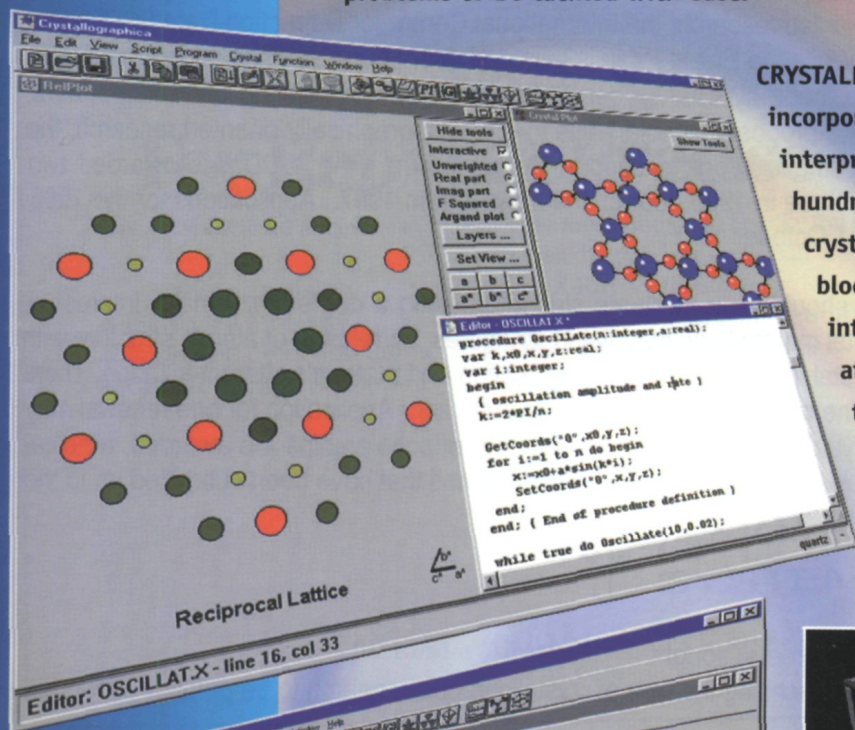
United Kingdom : Arthur Bagley  
 Hiltonbrooks Ltd.  
 Phone : 0 1477 534140  
 Fax : 0 1477 535041

All Trademarks are the properties of their respective owners

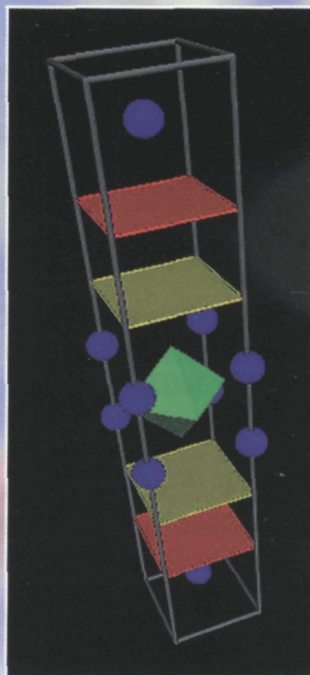


crystallographica

Introducing the ideal software toolkit for chemists, physicists, biotechnologists, mineralogists, and all material scientists with an interest in crystal properties. CRYSTALLOGRAPHICA combines the ease of use of a Microsoft Windows interface with the power of a programming language, allowing simple and complex problems to be tackled with ease.



CRYSTALLOGRAPHICA incorporates a Pascal interpreter extended with hundreds of crystallographic 'building block' routines. This is integrated with many attractive graphical tools to make CRYSTALLOGRAPHICA the perfect research and teaching aid.



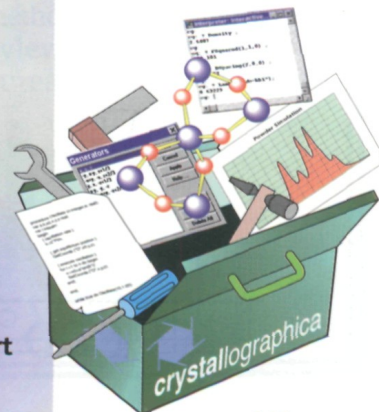
# crystallographica

For more information contact:  
**OXFORD  
CRYSTALLOGRAPHICA**

3 Blenheim Office Park  
Lower Road  
Long Hanborough · Oxford  
OX8 8LN · UK  
Tel. +44 (0)1993 883488  
Fax. +44 (0)1993 883988

email: sales@cgraph.demon.co.uk  
http://www.demon.co.uk/oxcryo  
(includes free demo version)  
Credit cards accepted

- Pascal interpreter with extensive library of crystallographic routines
- Integrated crystal structure drawing plus new VRML export
- New reciprocal lattice viewer with a variety of plotting styles
- X-ray and neutron powder pattern simulation
- Installation includes numerous example scripts and crystal structures
- Comprehensive printed and on-line help, plus technical support



# INTERNATIONAL CENTRE FOR DIFFRACTION DATA CRYSTALLOGRAPHY SCHOLARSHIP AWARDS

The science of crystallography has played a key role in the development of X-ray diffraction, electron diffraction and neutron diffraction for the elucidation of the atomic structure of matter. Crystallography is an interdisciplinary branch of science taught in departments of physics, chemistry, geology, molecular biology, metallurgy and material science. To encourage promising graduate students to pursue crystallographically-oriented research, the International Centre for Diffraction Data (ICDD) has established a Crystallography Scholarship Fund. While the Ewald Prize is awarded every three years to an internationally recognized crystallographer, little effort has been made by science departments to cultivate aspiring crystallographers. Convinced of the beneficial, scientific impact of the proposed scholarships for crystallographically-oriented research, the ICDD has solicited funds from private and industrial sectors to support this program. The ICDD has awarded two scholarships in 1992, two in 1993, three in 1994, three in 1995, four in 1996 and four in 1997. Applications for the 1998 awards must be received by ICDD no later than 31 October 1997.

**Qualifications for the applicants:** The applicant should be a graduate student seeking a degree with major interest in crystallography e.g. crystal structure analysis, crystal morphology, modulated structures, correlation of atomic structure with physical properties, systematic classification of crystal structures, phase identification and materials characterization. There are no restrictions on country, race, age or sex. The term of the scholarship is one year. Application for one renewal may be made by the recipient at the end of the first year. Because a limited number of scholarships are awarded, renewal applications will be considered on a competitive basis in conjunction with all applications that have been submitted up to the closing date.

**Submit:**

- a. Curriculum Vitae, listing degree(s) held and degree(s) sought.
- b. A one-page proposal by the graduate student describing the type of crystallographic research to be partially supported by scholarship.
- c. A supportive letter from the sponsoring professor of an accredited university or an institute of technology on institution letterhead.

**Restrictions on the scholarship fund:**

- a. The scholarship stipend of \$2,000 is to be used by the graduate student to help defray tuition and laboratory fees. A portion of the stipend may be applied to registration fees to accredited scientific meetings related to crystallography.
- b. No more than one scholarship will be awarded to applicants at any one accredited institution per year.
- c. The funds of the scholarship are not to be used for travel.

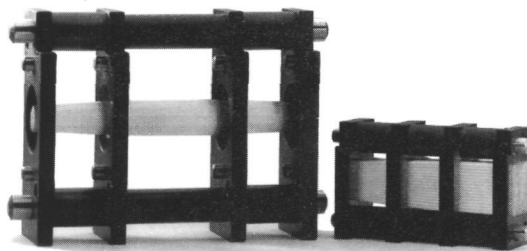
The awarding of the scholarships shall be administered by a committee consisting of the ICDD Chairman, the Chairman of the ICDD Technical Committee, the Chairman of the ICDD Education Subcommittee, and one or two individuals without conflict of interest. One or more accredited professors (with no conflicts of interest) may be invited to assist in the selection of successful candidates.

Applications must be received by 31 October 1997. Please mail to:

Secretary, International Centre for Diffraction Data  
12 Campus Boulevard  
Newtown Square, PA 19073-3273 U.S.A.



Focusing lens with large collection angle and focal spot of down to 50  $\mu\text{m}$  FWHM, accurately directs x-ray energies from 200 eV to 30 KeV.



Collimating lens collects large solid angles and produces low divergence, well collimated beam.

## New X-Ray Lenses For Rapid & Precise Measurements.

Need speed and accuracy in critical x-ray measurements? Specify the only commercially available polycapillary optics.

Get real bottom line savings in time and money.

- |                                                                                                                                                                                 |                                                                                                                                                                                                                      |                                                                                                                                                      |                                                                                                                                   |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------|
| <p><b>X-Ray Focusing</b></p> <ul style="list-style-type: none"> <li>▲ Increased intensity</li> <li>▲ Improved detection limits</li> <li>▲ Greater spatial resolution</li> </ul> | <p><b>X-Ray Collimating</b></p> <ul style="list-style-type: none"> <li>▲ Two dimensional collimation</li> <li>▲ More efficient use of source for increased total flux</li> <li>▲ Broad spectral bandwidth</li> </ul> | <p><b>Diffraction Applications</b></p> <ul style="list-style-type: none"> <li>▲ Texture</li> <li>▲ Stress</li> <li>▲ Phase identification</li> </ul> | <p><b>Fluorescence Applications</b></p> <ul style="list-style-type: none"> <li>▲ Composition</li> <li>▲ Film thickness</li> </ul> |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------|

Have a polycapillary optics application? Call Phil Bly, our Sales and Applications Engineer.

It could be the most productive call you'll make this year.



**X-RAY  
OPTICAL  
SYSTEMS  
INC.**

90 Fuller Road • Albany, NY 12205 • 518/ 442-5250 PH • 518/ 442-5292 FAX  
pbly@xos.com www.xos.com

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

### Fundamentals of X-ray Powder Diffraction

June 1-5, 1998

Emphasizing instrumentation, specimen preparation, data acquisition, and qualitative phase analysis.

### Advanced Methods in X-ray Powder Diffraction

June 8-12, 1998

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

### Fundamentals of X-ray Fluorescence

April 20-24, 1998

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.

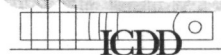
### Advanced Methods in X-ray Fluorescence

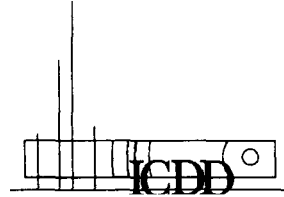
April 27-May 1, 1998

Emphasizing quantitative methods, use of automated X-ray 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, e-mail: CLINICS@ICDD.COM

**International Centre for Diffraction Data**





## Publishing Agreement

1. It is our custom to request authors to vest the worldwide copyright of their papers with the JCPDS—International Centre for Diffraction Data for the full term of copyright and we would be grateful if you would confirm your acceptance of these terms by signing and returning the agreement below. We will not withhold permission for any reasonable request from you to publish any part of this paper in connection with any other work by you, provided the usual acknowledgements are given regarding copyright notice and reference to the original publication.
2. If it is appropriate, the author's employer may sign this agreement, and in any event the employer may reserve the right to use the paper internally or for promotional purposes only, by so indicating on this agreement. It is understood that proprietary rights other than copyright (including patent rights) are reserved.
3. If the author is a U. S. Government employee and this work was done in that capacity the assignment applies only to the extent allowable by U. S. law. If at least one co-author is *not* a government employee, said author should sign the agreement.
4. If the author is an employee of the British Government then HMSO will grant a non-exclusive license to publish this paper in the Journal in any form or media provided British crown copyright and user rights (including patent rights) are reserved.
5. The author warrants that the manuscript is the author's original work, and has not been published before. (If excerpts from copyrighted works are included, the author will obtain written permission from the copyright owners and show credit to the sources in the manuscript.) The author also warrants that the article contains no libelous or unlawful statements, and does not infringe on the rights of others.
6. If the work was prepared jointly the author agrees to inform co-authors of the terms of the agreement, and to sign on their behalf.

---

With the qualifications listed above I assign to JCPDS—International Centre for Diffraction Data, the copyright of my paper entitled

---

---

for publication in *Powder Diffraction*.

\_\_\_\_\_  
Signed

\_\_\_\_\_  
Date

If the paper is rejected, this assignment is null and void.