



# Powder Diffraction

*An international  
journal of materials  
characterization*

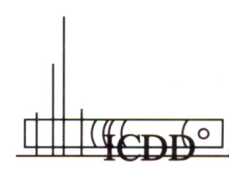
Volume 15 Number 3 September 2000

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

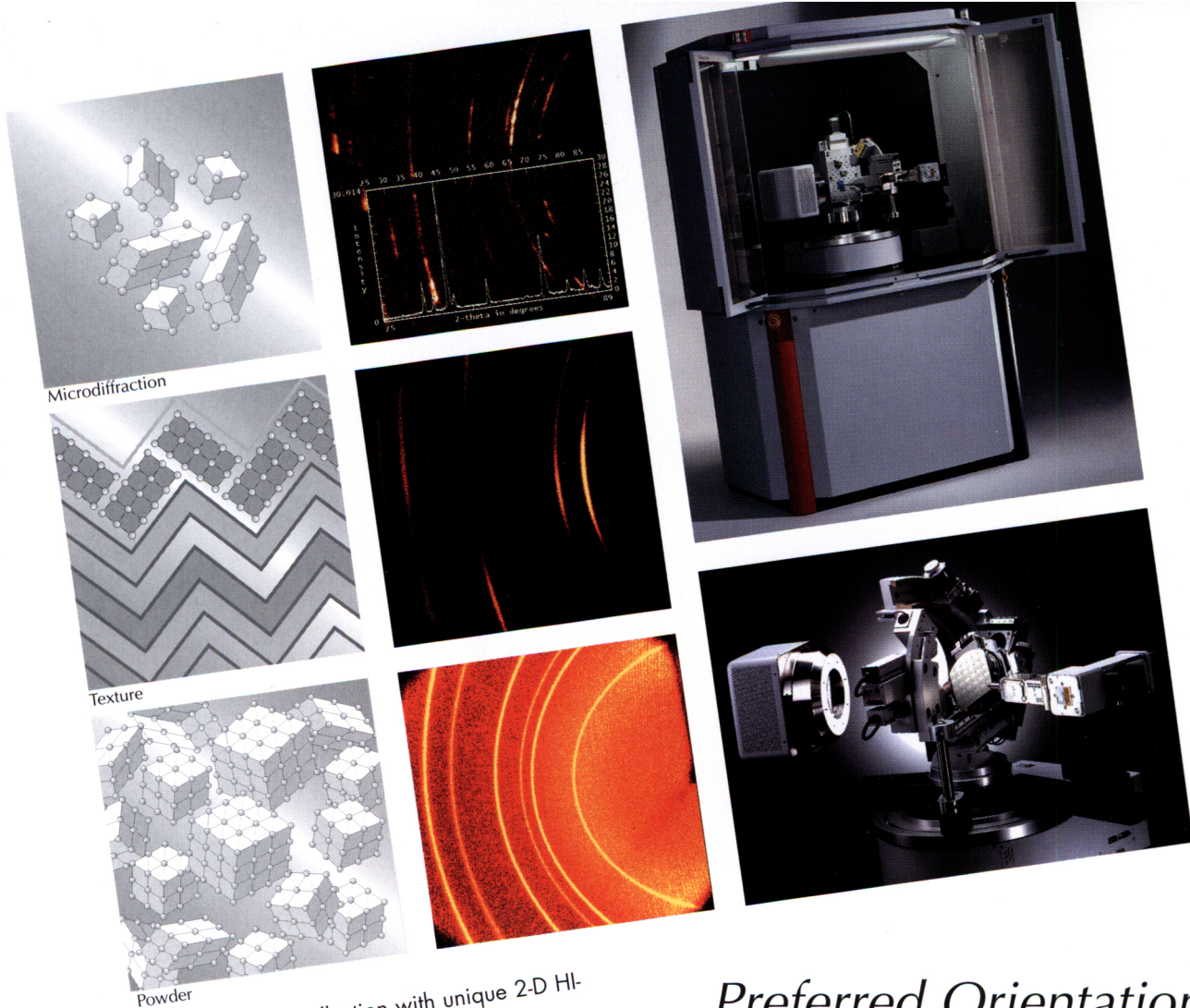
Rad. CuKα <sub>1</sub> Cut off	λ 1.40598 Int. Diffractometer	Filter Mono. d-sp Diff. I/L <sub>α</sub> 3.6	dÅ	Int	hkl	dÅ	Int	hkl	★
			4.257	22	100	1.1532	1	311	
			3.342	100	101	1.1405	<1	204	
			2.457	8	110	1.1143	<1	303	
			2.282	8	102	1.0813	2	312	
			2.237	4	111	1.0635	<1	400	
			2.127	6	200	1.0476	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	105	
			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	114				
			1.1804	3	314				
				3	314				

Ref. Natl. Bur. Stand. (U.S.) Monogr. 25, 18 61 (1981)  
S.G. P3,21 (154)  
c 5.4053(4) Å  
Z 3 mp C 1.1001  
SS/FOM F<sub>w</sub>=77(.013,31)  
Sign + 2V  
Ref. Swanson, Fuyat, Natl. Bur. Stand. (U.S.), Circ. 539, 3 24 (1954)

Color Colorless  
Pattern taken at 25 C. Sample from the Glass Section at NBS, Gaithersburg, Maryland, USA, ground single-crystals of optical quality. Pattern reviewed by Holzer, G., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA, ICDD Grant-in-Aid (1990). Agrees well with experimental and calculated patterns. O<sub>2</sub>Si type. Quartz group. Also called: silica. Also called: low quartz. Silicon used as internal standard. PSC: hP9. To replace 5-490 and validated by calculated pattern. Plus 6 additional reflections to 0.9089.







Microdiffraction

Texture

Powder

- Real-time data collection with unique 2-D HI-STAR detector
- Lowest background level for highest signal sensitivity
- Simultaneous large  $\chi$  and  $2\theta$  data acquisition for fastest powder and texture investigations
- 2-D texture, residual stress, and microdiffraction with incomparable quality
- Small Angle X-ray Scattering capability for 2-D large structure examination
- Cross-coupled Göbel Mirrors for highly intense, point like parallel beam
- Comprehensive range of stages for every kind of sample
- Sophisticated laser/video system for easy sample alignment and positioning
- GADDS and DIFFRAC<sup>plus</sup> software suite for every kind of application
- Unrivaled flexibility and versatility inherent in the D8 diffraction family

*Preferred Orientation,  
Microdiffraction,  
Grained Materials,  
Large Structures...*

...perfect for  
**D8 DISCOVER**  
with GADDS

**find out  
what's inside**

**BRUKER ADVANCED X-RAY SOLUTIONS**



Worldwide: Tel. (+49) 721/595-2888 • Fax (+49) 721/595-4587 • <http://www.bruker-axs.de> • E-mail: [info@bruker-axs.de](mailto:info@bruker-axs.de)  
USA and Canada: Tel: (+1) 608/276-3000 • Fax: (+1) 608/276-3006 • <http://www.bruker-axs.com> • E-mail: [info@bruker-axs.com](mailto:info@bruker-axs.com)





# crystallographica searchmatch

The makers of *Crystallographica* are proud to announce the launch of *Crystallographica Search-Match*, an all-new search-match program for Windows 95/98/NT.

- ◆ Works with all versions of the Powder Diffraction File including the new cPDF
- ◆ Search using full powder diffraction pattern and/or peak list
- ◆ Automatic residual search for multi-phase identification
- ◆ Unique integrated Boolean card retrieval and display
- ◆ Single / multi-phase full pattern powder simulations
- ◆ Reads common file formats
- ◆ Built-in tools include peak finding and background /  $k\text{-}\alpha_2$  stripping
- ◆ Report writing directly to Microsoft Word
- ◆ Full 32-bit technology delivering unrivalled speed and power

Visit our new web site for details  
or contact us for a free demo CD!



OxfordCryosystems

3 Blenheim Office Park, Lower Road, Long Hanborough  
Oxford · OX8 8LN · UK

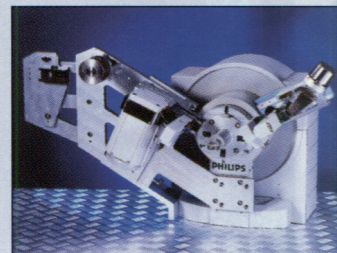
Tel: +44 (0)1993 883488 · Fax: +44 (0)1993 883988  
E.mail: info@OxfordCryosystems.co.uk

[www.crystallographica.co.uk](http://www.crystallographica.co.uk)

## Search-Match? Upgrade to the state-of-the-art



# X-ray diffraction for today and tomorrow



The inevitability of change has long been recognized - and the pace of change is accelerating at an ever increasing rate. This is true in the laboratory domain as in every other aspect of modern life. What you require from your X-ray diffractometer could be a world apart from your expectations today.

The Philips X'Pert PRO diffractometer system is an X-ray diffraction system with a virtually limitless capacity to adapt to changing circumstances. the PreFIX (Pre-aligned, Fast-Interchangeable X-Ray optics) system enables instruments to be reconfigured in a few minutes to handle different types of analysis.

A totally open design architecture guarantees full freedom to accommodate further advances in years to come.

**For more information:**  
Philips Analytical  
Lelyweg 1,7602 EA,  
Almelo, The Netherlands  
Tel. : +31 (546) 534444  
Fax : +31 (546) 534592

[www.analytical.philips.com](http://www.analytical.philips.com)

*Let's make things better.*

Published online by Cambridge University Press



**PHILIPS**



**Editor-in-Chief**

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

**Managing Editor**

Shannon Mataboni  
JCPDS-International Centre for Diffraction Data  
12 Campus Blvd.  
Newtown Square, PA 19073-3273 U.S.A.  
mataboni@icdd.com

**Editor for Reviews and Reprints**

Deane K. Smith  
1652 Princeton Drive  
State College, PA 16803-3273 U.S.A.  
smithdeane@aol.com

**Editor for New Diffraction Data**

William E. Mayo  
Rutgers University  
Ceramics Department  
Piscataway, NJ 08855-0909 U.S.A.  
edisonjam@aol.com

**Western European Editor**

Norberto Masciocchi  
Università di Milano  
Dipartimento di Chimica  
Strutturale e Stereochimica Inorganica  
Via Venezian, 21  
20133 Milano, Italy  
norbert@csmtbo.mi.cnr.it

**Eastern European Editor**

Jaroslav Fiala  
SKODA Research Ltd.  
31600 Plzeň, Czech Republic  
jaroslav.fiala@vsb.cz

**Editor for Southeast Asia**

Brian H. O'Connor  
Curtin University  
GPO Box U 1987, Perth 6001  
Western Australia, Australia  
toconnorb@cc.curtin.edu.au

**Editor for Japan**

Hideo Toraya  
Ceramics Research Lab  
Nagoya Institute of Technology  
Asahigaoka, Tajimi 507 Japan  
toraya@crl.nitech.ac.jp

**International Reports Editor**

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

**Editorial Advisory Board**

P. Bayliss, Sydney, Australia  
C. Z. Bojarski, Katowice, Poland  
A. Brown, Dorset, England  
D. Cox, Upton, New York  
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  
T. Yamanaka, Tokyo, Japan  
R. A. Young, Atlanta, Georgia

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

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

**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, Suite 1N01, 2 Huntington Quadrangle, Melville, NY 11747-4502.

**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, Suite 1N01, 2 Huntington Quadrangle, Melville, NY 11747-4502; phone: (516) 576-2440; fax: (516) 576-2481.

**Subscription Prices (2000)**

	U.S.A & Canada	Mexico, Central & South America	Europe, Mid-East & Africa*	Asia & Oceania*
Individual	\$60	\$85	\$85	\$85
Institutional or Library	\$105	\$105	\$105	\$105

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

**Back-Number Prices.** 2000 single copies: \$30. Prior to 2000 single copies: \$30.

**Subscription, renewals, and address changes** should be addressed to *AIP Circulation and Fulfillment Division (CFD)*, Suite 1N01, 2 Huntington Quadrangle, Melville, NY 11747-4502. 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, Melville, NY 11747-4502; (516) 576-2230; (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 0885-7156/2000 \$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, Suite 1N01, 2 Huntington Quadrangle, Melville, NY 11747-4502; Fax: 516-576-2450; Telephone: 516-576-2268; E-mail: rights@aip.org.

**Document Delivery:** Copies of journal articles can be ordered for online delivery from DocumentStore, AIP's online document delivery service (<http://ojps.aip.org/documentstore/>).

**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, Suite 1N01, 2 Huntington Quadrangle, Melville, NY 11747-4502; Fax: 516-349-9704; Telephone: 800-344-6909 (in U.S. and Canada), or 516-576-2234.

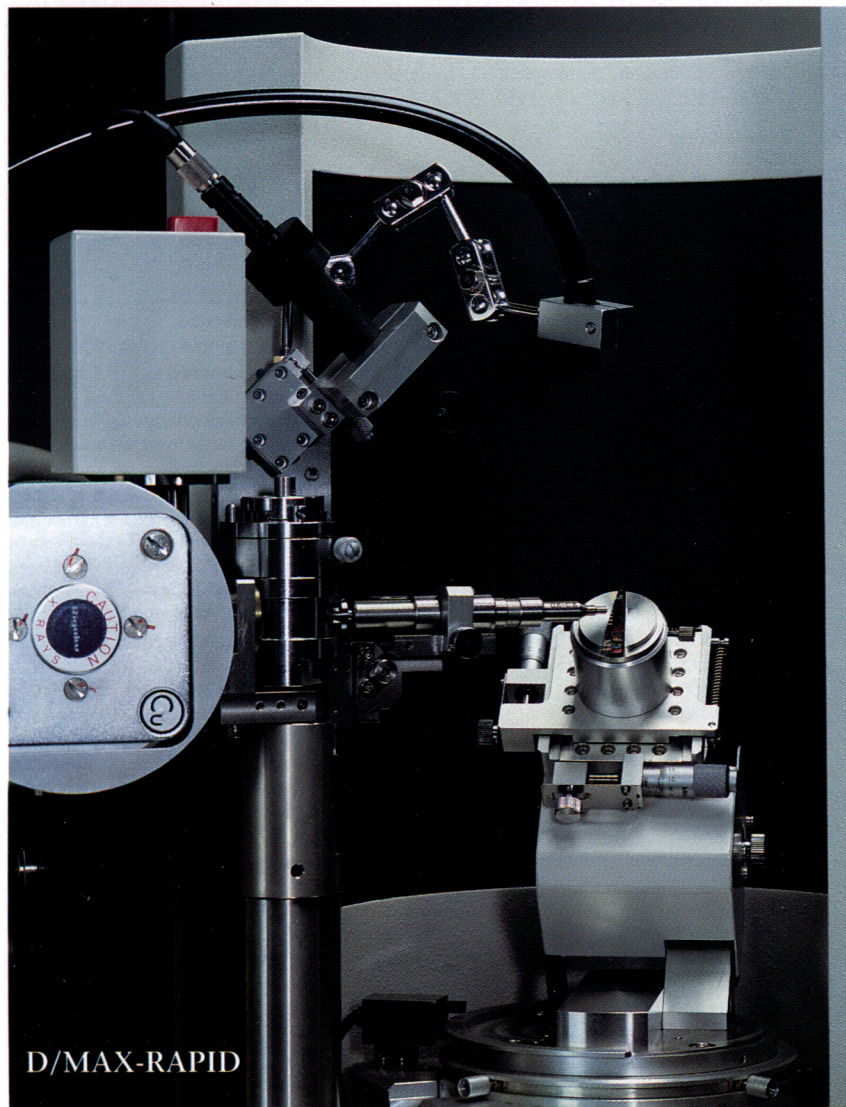
*Powder Diffraction* (ISSN: 0885-7156) is published quarterly (4X annually) by the JCPDS-International Centre for Diffraction Data through the American Institute of Physics. 1999 Subscription rates: US\$105. POSTMASTER: Send address changes to *Powder Diffraction*, AIP Circulation & Fulfillment Division, Suite 1N01, 2 Huntington Quadrangle, Melville, NY 11747-4502. Periodicals postage paid at Huntington Station, NY 11746, and additional mailing offices.

**Online Availability:** Abstracts of journal articles published by the AIP and Member Societies (and several other physics publishers) are available from AIP's SPIN database, via AIP's Online Journal Publishing Service (OJPS) (<http://ojps.aip.org>).

**Copyright © 2000 JCPDS-International Centre for Diffraction Data, 12 Campus Blvd., Newtown Square, PA 19073-3273. All rights reserved.**  
[www.icdd.com/products/journals.htm](http://www.icdd.com/products/journals.htm)



# 0-160 *in 12 seconds..!*



## **High-sensitivity High-resolution Curved Image Plate Microdiffraction System**

Rigaku presents another technological breakthrough with the D/MAX-RAPID microdiffraction system. The D/MAX-RAPID's curved image plate technology offers higher sensitivity, higher resolution, higher speed and larger area mapping compared to traditional multiwire and CCD technology.

In reflection mode, a 0-160° 2 $\theta$  image obtained with an average azimuthal angle of 30° can be collected **in 12 seconds** with an optional ultraX rotating anode. The D/MAX-RAPID covers large areas of the Debye cones with its 465mm by 256mm image plate.

The system can be used with Cu, Mo, Cr, or Co X-ray sources and can be configured with either sealed tube X-ray generators or with the Rigaku ultraX 18kW rotating anode generator. With a high-dynamic range of 1 x 10<sup>6</sup>, the D/MAX-RAPID overcomes the limitations of other 2-D detectors.

### **Advanced features of the D/MAX-RAPID include:**

- Fast phase identification
- Polymer and fiber diffraction
- Texture and orientation
- Percent crystallinity
- Crystallite size
- Microdiffraction
- Selected-area diffraction (Diffraction-function mapping)
- Stress
- Forensics
- Inclusions
- High-pressure diamond anvil studies
- Single crystal diffraction (with optional single crystal software/hardware package)

**Rigaku**

9009 New Trails Drive  
The Woodlands, TX 77381  
Tel: (281) 367-2685  
Fax: (281) 364-3628  
<http://www.rigaku.com/pd>



## EDITORIAL

- Ting C. Huang International X-ray Analysis Society (IXAS) forms in Barcelona 161

## TECHNICAL ARTICLES

- Ryan S. Winburn, Dean G. Grier, Gregory J. McCarthy, and Renee B. Peterson Rietveld quantitative X-ray diffraction analysis of NIST fly ash standard reference materials 163
- Wu Wanguo, Ruan Yuzhong An external standard method for angular calibration of powder diffractometers 173
- B. Barbier, H. Euler X-ray powder diffraction data for calcium galactarate tetrahydrate  $\text{CaC}_6\text{H}_8\text{O}_8 \cdot 4\text{H}_2\text{O}$  and Rietveld refinement of the crystal structure 175

## NEW DIFFRACTION DATA

- Gabriella Salviulo, Giovanni B. Andreozzi, and Giorgio Graziani X-ray characterization of Mg, Fe, and Mn natural end-members of the axinite group 180
- D. Sornadurai, B. Panigrahi, V. S. Sastry, and Ramani Crystal structure and X-ray powder diffraction pattern of  $\text{Ti}_2\text{ZrAl}$  189
- Luz Amparo Palacio, Carlos Saldarriaga X-ray powder diffraction data for zinc molybdate,  $\text{Na}(\text{OH})\text{Zn}_2(\text{MoO}_4)_2 \cdot 2.5\text{H}_2\text{O}$  191
- V. Venegas, G. Rueda-Morales, E. Reguera, and F. Caleyó Structural characterization of dimercury( $1^+$ ) pentacyanonitrosylferrate( $2^-$ ),  $\text{Hg}_2[\text{Fe}(\text{CN})_5\text{NO}]$  193

## LETTER TO THE EDITOR

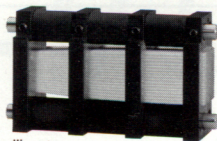
- Jeffrey E. Post Comment on "Status of the reference X-ray powder diffraction patterns for the serpentine minerals in the PDF database—1997," by Fred J. Wicks [Powder Diffr. 15, 42–50 (2000)] 198

## INTERNATIONAL REPORTS

- Regional Reports 199
- Book Review 202
- Calendar of Meetings 203
- Short Courses & Workshops 207
- Cumulative Author Index 209

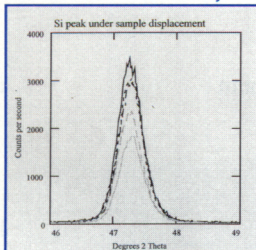


Enhance instrument **PERFORMANCE** with X-ray collimating lenses for parallel beam powder diffraction from **X-RAY OPTICAL SYSTEMS.**

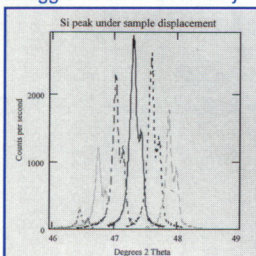


x-ray collimator  
(10x10 mm<sup>2</sup> output beam)  
©XOS 1996

Parallel Beam Geometry



Bragg-Brentano Geometry



Outstanding Performance in **Stress and Texture Applications**

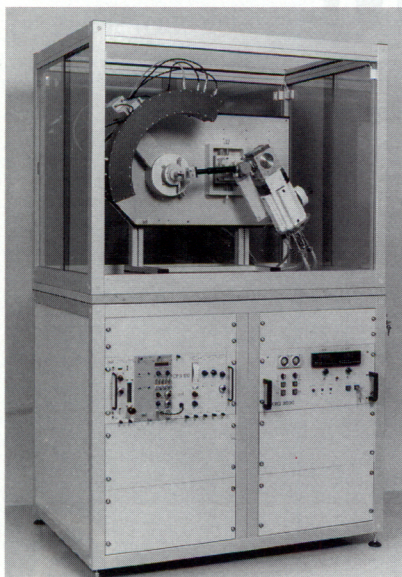
Elimination of all defocusing errors	No sample preparation needed
Large beam size	Improved particle statistics
Intensity gain up to 40 X	Improved counting statistics
2-D collimated quasi parallel beam	Increased orientation statistics
Constant peak profile and width over whole 2 $\theta$ range	Ideally suited for industrial applications and full pattern analysis

Also available, X-ray focusing lenses for Micro X-Ray Fluorescence.  
Call J.Phillip Bly, Sales and Application Engineer today.



30 Corporate Circle • Albany, NY 12203  
Phone: 518.464.3334 • Fax: 518.464.3335  
www.xos.com • email: info@xos.com

# inel REAL TIME XRD



MPD Multi-Purpose X-ray  
Diffractometer

Versatile diffractometers designed to take advantage of the rapid, real time data collection our patented CPS X-ray detectors offer.

- \*No scanning feature - acquire up to 120° 2 $\theta$  simultaneously
- Unique capillary devices for analysis of air sensitive materials
- Identify materials even if only micro amounts are available
- Parallel beam with germanium or multilayer mirror optics

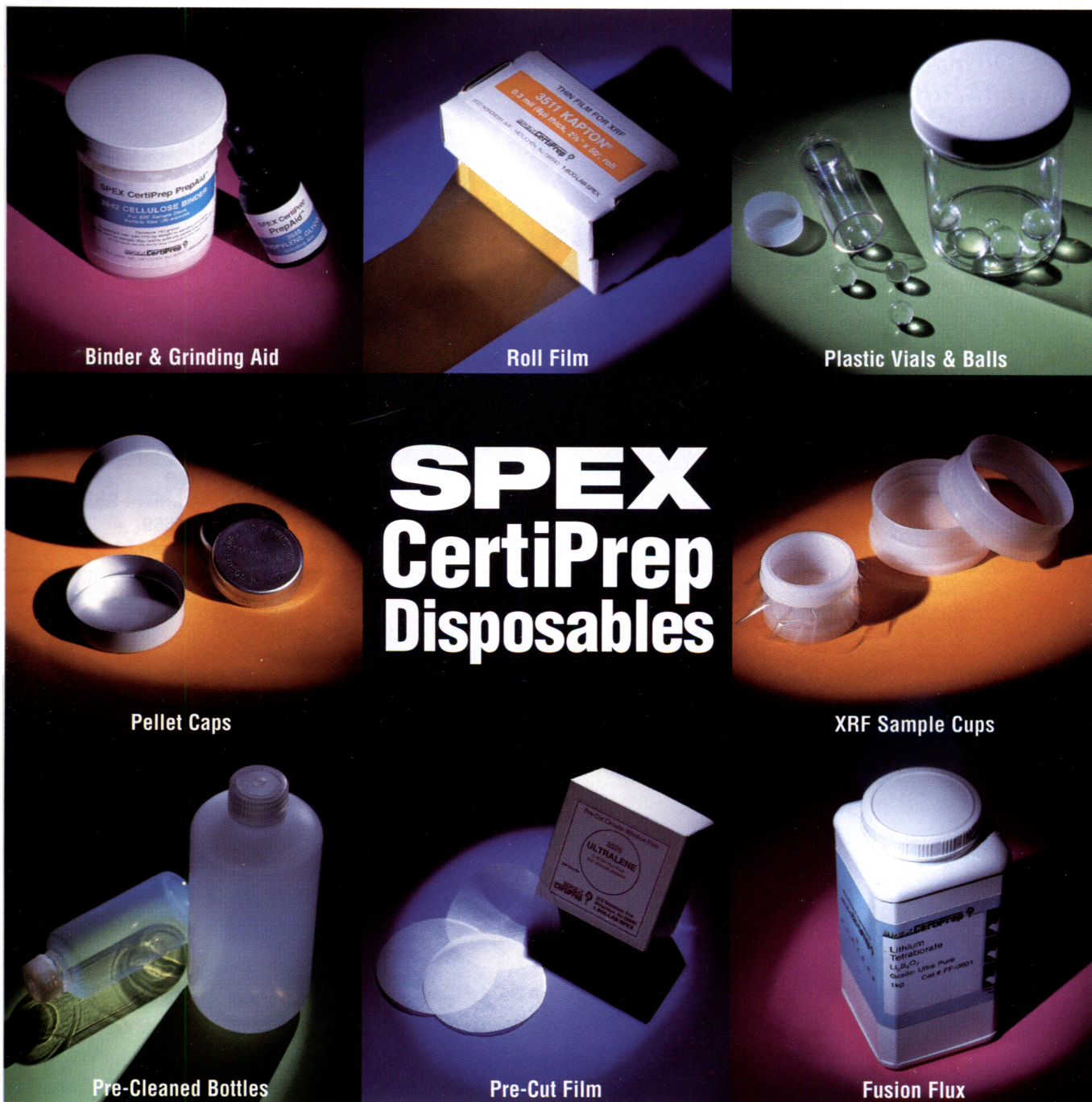
*for information on our complete product line please contact us*

**inel** - Z.A - CD 405 - 45410 ARTENAY (FRANCE)  
Tel. (33) 0 2 38 80 45 45 Fax. (33) 0 2 38 80 08 14  
E.MAIL: inel@valcofim.fr-INTERNET:<http://www.valcofim.fr/inel>

**inel Inc.** P.O. Box 147, STRATHAM, NH 03885 (USA)  
TEL. (603) 778-9161 FAX. (603) 778-9171  
E-MAIL: inelinc@aol.com



# 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 ■ 732-549-7144  
Fax 732-603-9647 ■ SamplePrep@spexcsp.com ■ <http://www.spexcsp.com>



# Traces v6

One of the world's most popular Powder Diffraction Scan Processing packages has a host of new features:

## Diffraction Technology

For all your X-ray Diffraction needs!

With instant access to all common functions with the right mouse button for instance, Traces v6 is one of the most user - friendly packages around!

Integrated Peak Fitting, Quantitation, Search/Match, Database access & creation, Indexing, Unit Cell refinement available as standard or option, also makes it great value for money

Visit our Website & download a Demo copy for yourself

[www.difftech.com.au](http://www.difftech.com.au)

Australia: Rod Clapp  
Diffraction Technology Pty Ltd  
PO Box 444 Mitchell A.C.T 2911  
Canberra, Australia.  
Ph: 61 2 6242 8233 / Fax: 61 2 6242 8266  
Email: [difftech@difftech.com.au](mailto:difftech@difftech.com.au)

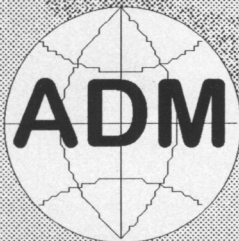
United Kingdom: Arthur Bagley  
Hiltonbrooks Ltd  
Ph: 0 1477 534140 / Fax: 0 1477 535041  
Internet: [arthur@xrays.u-net.com](mailto:arthur@xrays.u-net.com)

USA: Jerry Krause  
Analytical X-ray Instrument Sales  
Phone/Fax: 303-277 1569  
Internet: [jkxray@aol.com](mailto:jkxray@aol.com)

Degrees 2-Theta

## Your Software For X-Ray Analysis

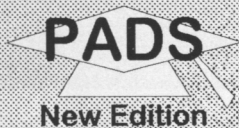
Now optimized for the new, enhanced PDF database with more than 42,000 additional calculated patterns



Software package for data acquisition and analysis:

Diffraction control, plot modules, peak search and calibration, qualitative and quantitative phase analysis, profile fitting and pattern simulation, lattice parameter refinement, crystallite size and micro stress.

Ready to plug to your PHILIPS and SIEMENS diffractometer hardware.



Stand alone package for qualitative and quantitative phase analysis.

Extremely fast search algorithms for ICDD-PDF database and user created databases. Very exact quantitative analysis using the WHOLE PATTERN method.



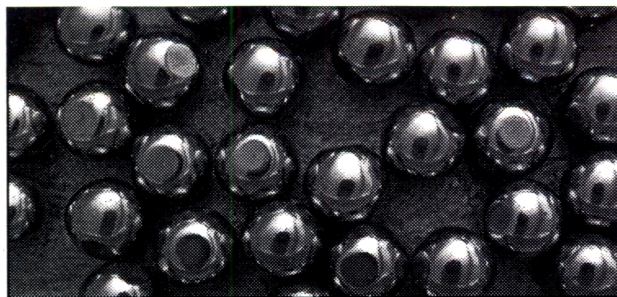
Extension package for most third party X-ray software. Graphic-analytical, profile-analytical and crystallographic options.

**a. wassermann**

*röntgenanalytik.meßsysteme.software*

P.O. BOX 2631, D-87416 Kempten, Germany, Tel. (49)0831-79515, FAX (49)0831-79930, E-mail: [RMSKempten@aol.com](mailto:RMSKempten@aol.com)





**NEW**  
**Speciality Products**  
from the **ICDD**<sup>®</sup>

**Introducing**  
relational database formatting  
for our specialty products

**Initial RDB release—  
Metals & Alloys!**

**RDB** formatting  
allows for extraordinary  
flexibility in data transmission  
as well as improved display  
and search capabilities.  
Enhanced data-mining along with  
affordable pricing makes the **RDB** an  
exceptional tool for your lab!

International Centre for Diffraction Data  
12 Campus Boulevard  
Newtown Square, PA 19073-3273 U.S.A.  
Sales: 610.325.9810  
Fax: 610.325.9823  
info@icdd.com  
www.icdd.com



Orders may be placed on-line via:  
[www.icdd.com/products](http://www.icdd.com/products)



International Centre for Diffraction Data

**ICDD POWDER SUITE**

*Support Software for  
The Powder Diffraction File*<sup>™</sup>



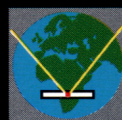
**PCPDFWIN**<sup>™</sup>  
**Windows**<sup>®</sup> Retrieval Software

Allows Windows<sup>®</sup> accessibility for PDF-2

Displays and prints multiple PDF<sup>®</sup> records

Search capabilities with filters and  
Boolean operators

Save research results to a file



**PCSIWIN**<sup>™</sup>  
**Search Index for Windows**<sup>®</sup>

PC alternative to printed Indexes and  
Search Manual

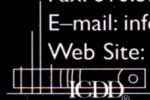
Performs Hanawalt & Fink Searches

Elemental subfile filters

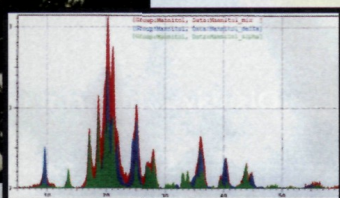
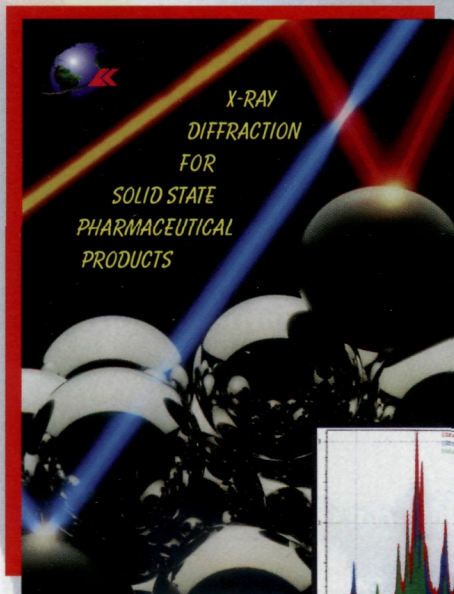
Boolean operator options

Visit us at [www.icdd.com](http://www.icdd.com)

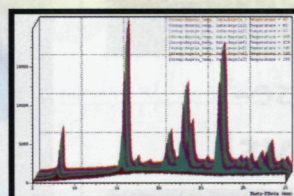
International Centre for Diffraction Data  
12 Campus Boulevard  
Newtown Square, PA 19073-3273 U.S.A.  
Technical: 610.325.9814 Sales: 610.325.9810  
Fax: 610.325.9823  
E-mail: [information@icdd.com](mailto:information@icdd.com)  
Web Site: [www.icdd.com](http://www.icdd.com)



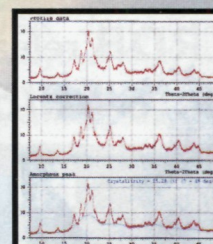




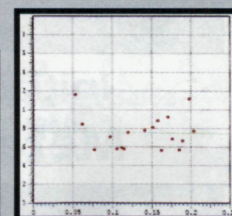
**PHASE ANALYSIS**  
65/45 MIX OF ALPHA & DELTA  
POLYMORPHS OF MANNITOL



**NON-AMBIENT STUDY**  
ASPIRIN OVER A TEMPERATURE  
RANGE OF 40°C - 180°C STEPS



**PERCENT CRYSTALLINITY**  
CALCULATED BY TOTAL  
PATTERN FITTING



**FULL PATTERN HALL METHOD**  
SHOWING VARIATION OF  
CRYSTAL SIZE



X-Ray Diffraction is a unique analytical tool for solid state pharmaceutical products to unambiguously characterize their solid state nature. Many parameters required by the FDA, legal patent issues and drug performance are only accessible by utilizing X-Ray Diffraction.

X-Ray Diffraction is a direct result of crystal structures being present in the pharmaceutical under study. As such, the parameters typically associated with crystal structure can be simply assessed. For example, once an active drug has been isolated, an indexed X-Ray powder diffraction pattern is required to secure a patent and protect a company's investment. Additionally, analysis of the drug under most environmental conditions reveals the formation of any polymorphs which could adversely effect the drug's performance and toxicity.

With the introduction of new systems specifically designed for the pharmaceutical industry, Kratos and Shimadzu have made X-Ray Diffraction cost effective and easy to use.

### XRD-6000 Designed for Pharmaceutical Research

- ◆ Polymorph Screening
- ◆ Percentage Crystallinity
- ◆ Morphology
- ◆ Crystal Structure Analysis
- ◆ Excipient Quantification
- ◆ Non-Ambient & Humidity Variation

Call or Write Today for More Information:



Kratos Analytical, Inc.

Phone: (914)426-6700

E-Mail: [info@kratos.com](mailto:info@kratos.com)

Internet: <http://www.kratos.com>

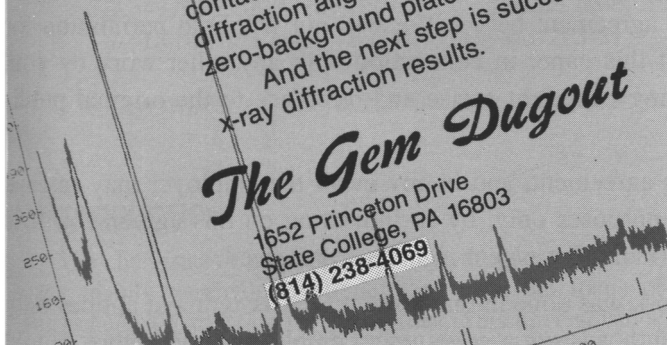
Call Today to Request Your Copy of  
*X-Ray Diffraction for  
Solid State Pharmaceutical Products*

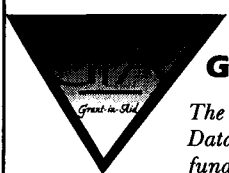


**X-ray  
Diffraction  
Reference Standards  
and Zero-background  
Sample Plates  
Custom Designed  
and Built for any  
Application**

Your first step to improved x-ray diffraction results should be to contact The Gem Dugout for quality diffraction alignment standards and zero-background plates. And the next step is successful x-ray diffraction results.

**The Gem Dugout**  
1652 Princeton Drive  
State College, PA 16803  
(814) 238-4069





**The ICDD's  
Grant-in-Aid Program**

*The International Centre for Diffraction Data (ICDD®) has increased grant-in-aid funding for the 2000–2001 grant cycles in order to allow more grants to be supported.*

---

The ICDD® is interested in high quality experimental powder diffraction patterns to add to its internationally renowned database, the Powder Diffraction File™ (PDF®). The ICDD's Grant-in-Aid Program is designed to give limited financial support to those institutions interested in supplying new patterns. A grant can be used most effectively as a supplement to existing funded projects involving the preparation and characterization of new materials, using powder XRD.


There are two grant cycles with proposal deadlines of:

Cycle I	31 January
Cycle II	31 July

---

For more information, please review the guidelines found on the ICDD® web site, <http://www.icdd.com>, or contact:

Ms. Shelley Wolkov, Grant Coordinator  
International Centre for Diffraction Data  
12 Campus Boulevard  
Newtown Square, PA 19073-3273 U.S.A.  
Phone: 610.325.9814 Fax: 610.325.9823  
E-mail: [WOLKOV@ICDD.COM](mailto:WOLKOV@ICDD.COM)



International Centre for Diffraction Data

Introduces


**E-commerce**

Ordering ICDD® products has never been easier!

From the Powder Diffraction File™ to the ICDD Powder Suite, all ICDD® products are available at our online store.

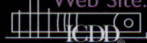
**The ICDD® Store offers:**

- Customer satisfaction
- Online order tracking
- E-mail order confirmation
- E-mail shipping notification
- Customer online order history
- Secure transmission using SSL encryption



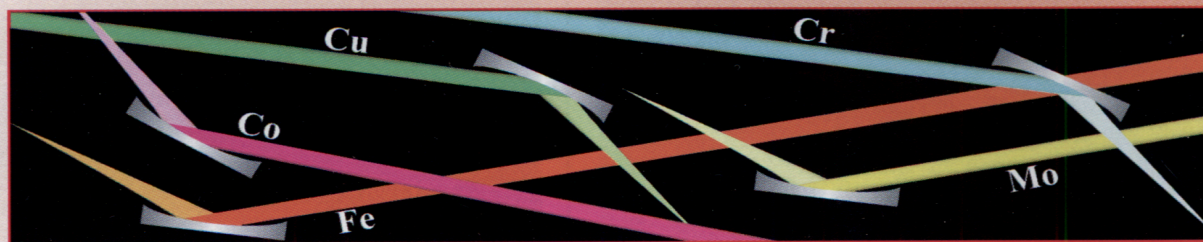
Visit us online at  
[www.icdd.com/products](http://www.icdd.com/products)

International Centre for Diffraction Data  
12 Campus Boulevard  
Newtown Square, PA 19073-3273 U.S.A.  
Technical: 610.325.9814 Sales: 610.325.9810  
Fax: 610.325.9823 E-mail: [information@icdd.com](mailto:information@icdd.com)  
Web Site: [www.icdd.com](http://www.icdd.com)

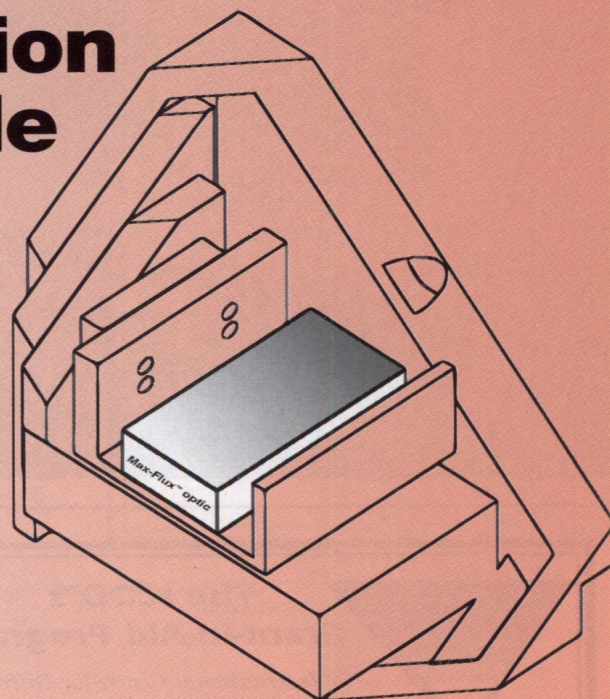
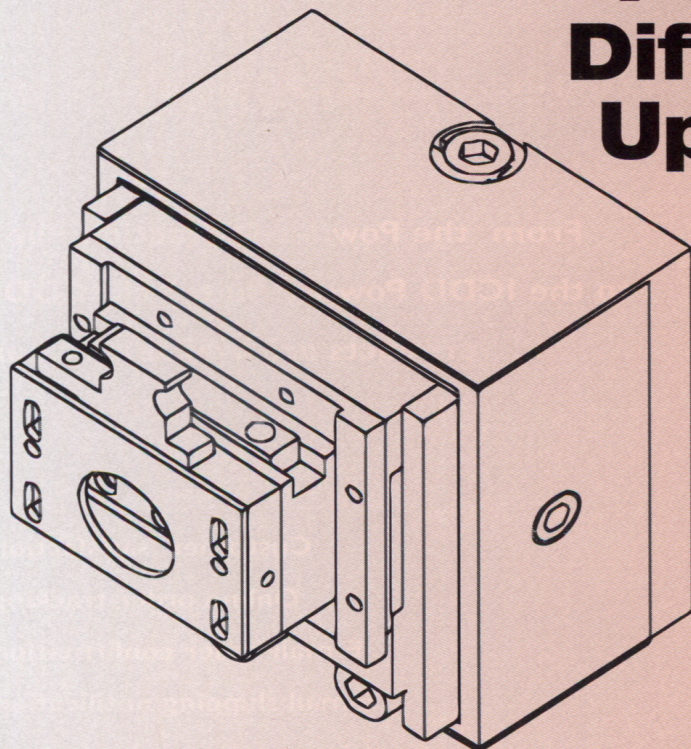




# Osmic Optics...



## Max-Flux™ Powder Diffraction Upgrade



### Benefits

- Reduction of sample displacement errors
- Enables testing of irregularly shaped samples
- Increased resolution
- Higher flux
- Lower background

### Applications

- Thin Film Analysis
- High Resolution
- Phase Analysis
- Stress / Strain Measurements
- Texture Analysis
- Point - Defect Analysis
- And more...

# Osmic Inc.

An Advanced Materials and Technology Company

1788 Northwood Drive  
Troy, Michigan 48084-5532, USA

tel: 248.362.1290

fax: 248.362.4043

[www.osmic.com](http://www.osmic.com)



The International Centre for Diffraction Data  
introduces

# Release 2000

of the

## Powder Diffraction File<sup>TM</sup>

the world's most complete X-ray powder diffraction pattern database!

### Experimental Patterns

- Over 85,000 experimental patterns compiled since 1941
- 2,500 new experimental patterns added for Release 2000

### Calculated Patterns

- Over 46,000 calculated patterns from the ICSD database
- 4,500 new calculated patterns added for Release 2000

### Editorial Integrity

- Dedication to detail and scientific purpose
- Four-tiered editorial process
- Highest standards for accuracy and quality

Visit us at [www.icdd.com](http://www.icdd.com)

International Centre for Diffraction Data

12 Campus Boulevard • Newtown Square, Pennsylvania 19073-3273 U.S.A.

Phone: 610.325.9814 • Sales: 610.325.9810 • Fax: 610.325.9823 • [info@icdd.com](mailto:info@icdd.com) • [www.icdd.com](http://www.icdd.com)

ICDD<sup>®</sup>



# ***SPEED***

IN POWDER DIFFRACTION

## **IMAGING PLATE GUINIER CAMERA 670\***

featuring the Low Temperature Device 670.4: Temperature range: 300 K...8 K



\* FAST, FLEXIBLE & FREE OF  $K\alpha_2$

**HUBER**  
X-RAY DIFFRACTION EQUIPMENT

HUBER Diffraktionstechnik GmbH  
Sommerstrasse 4  
D-83253 Rimsting  
Germany

Tel.: +49 (0) 80 51 - 68 78 - 0  
Fax: +49 (0) 80 51 - 68 78 - 10  
e-Mail: [info@xhuber.com](mailto:info@xhuber.com)  
URL: [www.xhuber.com](http://www.xhuber.com)