

Powder Diffraction

	Editorial	1
Davor Balzar, Hassel Ledbetter, and Alexana Roshko	X-ray diffraction peak-broadening analysis of $(\text{La-M})_2\text{CuO}_4$ high- T_c superconductors	2
R. Černý and V. Kupčík	Geometrical factors for correction of intensities in Seemann-Bohlin diffractometry	7
Vjera Novosel Radović	X-ray diffraction analysis of the cause of catalyst deactivation	14
K. D. Rogers and D. Cossins	An X-ray diffraction study of pyrolytic manganese dioxide	18
G. D. Yao and C. L. Kuo	A method of quantitative phase analysis using reference samples with absent phases	25
D. W. Tomlin, D. B. Sullenger, and J. S. Cantrell	A quantitative X-ray powder diffraction analysis of the $\text{Li}_2\text{O-SiO}_2$ glass-ceramic system	29
Liu Fengchao	Confirmation of the new technique for measuring the linear thermal expansion of silicon	36
Patricia Bénard, Jean Paul Auffrédic, and Daniel Louër	High-temperature X-ray powder diffractometry of the decomposition of zirconium hydroxide nitrates	39
Ludo K. Frevel and Cyrus E. Crowder	X-ray powder diffraction data for beryllonite from Stoneham, Maine, U.S.A.	47
Peter C. Burns and Frank C. Hawthorne	Rietveld refinement of the crystal structure of $\alpha\text{-CoSO}_4$	54
N. Guillou, J. P. Auffrédic, and D. Louër	Powder diffraction data for two mixed nitrates $\text{CeM}_2^{\text{I}}(\text{NO}_3)_6$ ($\text{M}^{\text{I}} = \text{Rb, Cs}$)	57
S. Katagiri, N. Ishizawa, and F. Marumo	A new high temperature modification of face-centered cubic Y_2O_3	60
Zhu Jinghuan, N. A. Raftery, and D. W. Field	X-ray diffraction powder data for Schlippe's salt $\text{Na}_3\text{SbS}_4 \cdot 9\text{H}_2\text{O}$	61
Jorge L. Garin and Rodolfo L. Mannheim	X-ray powder diffraction pattern of $\text{Mo}_{4.8}\text{Si}_3\text{C}_{0.6}$	65
	International Report	68
	Calendar of Meetings	68
	Computer Comments	69
	Commercial Announcements	70
	Cumulative Author Index	71



Volume 8 Number 1 March 1993

Powder Diffraction An international journal of materials characterization

SIEMENS

Is your diffraction system as flexible as you are?

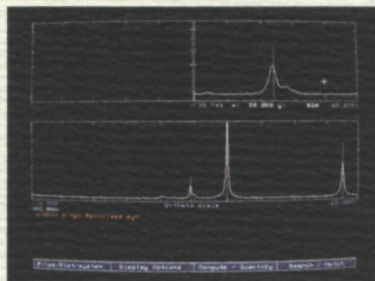
When the only thing you can count on in your lab is change, don't lock yourself in with a system designed to handle only some of your powder diffraction applications. If what you really need is flexibility, your options are open with the Siemens D 5000 X-ray diffractometer.

The modular D 5000 offers superior accuracy and speed with the most flexible and easy-to-learn software available worldwide. Most accessories can be installed or removed in minutes.

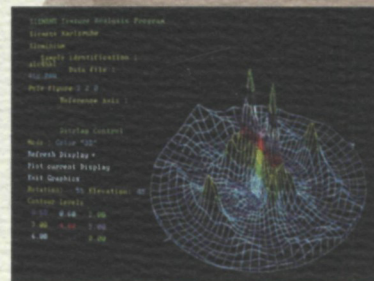
If flexibility is what you need, **Siemens delivers satisfaction.**



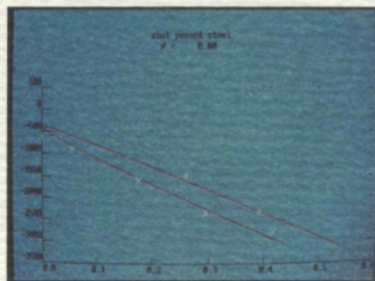
Raw data, full pattern phase analysis within the EVA2 graphics program.



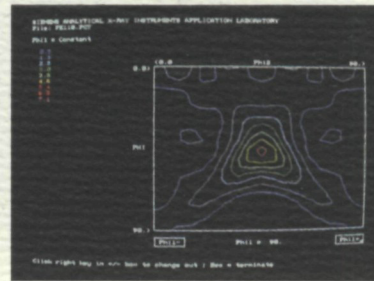
Flexible 3-D texture analysis software includes polefigure and constant phi displays.



Complete calculation of the full residual stress tensor using uniaxial, biaxial or triaxial stress calculations.



Orientation distribution function (ODF) evaluation software provides complete analysis of texture effects.



In USA & Canada contact: Siemens Analytical X-Ray Instruments, Inc. • 6300 Enterprise Lane • Madison, WI 53719 • (608) 276-3000
Worldwide contact: Siemens AG, Analytical Systems AUT V 371 • P.O. Box 21 1262 • D 7500 Karlsruhe 21 • Germany • (0721) 595-4295



Look into μ PDSM . . . It's more than accuracy. It's performance.

Performance makes μ PDSM the one search/match software system that approaches universality. It's the result of many years of research into putting all the complexities of qualitative XRD analysis in a single system for your personal computer—and now we've added graphics with a power that matches the unparalleled performance that established μ PDSM's reputation.

The utility of function and clarity of content in μ PDSM's graphics go beyond merely attractive presentation, to give you a valuable addition to the analytic power μ PDSM puts at your finger tips. With options that include fully integrated CD-ROM PDF-2 retrieval, direct instrument control, data acquisition, and diffractogram analysis, μ PDSM

gives you a flexibility of application to match the power of its performance.

The universal applicability and continuing enhancement of μ PDSM reflect the evolving technology of a company dedicated to software innovation. And you realize the results of Fein-Marquart's commitment to progress through a continuing update policy that keeps you at the state of the art.

Look into μ PDSM. It takes you beyond accuracy into the next generation of search/match performance.



Fein-Marquart Associates, Inc.
7215 York Road · Baltimore, MD 21212
(301) 821-5980

A1

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

We'll Help You Get A Handle On Your Sample

The SPEX Handbook includes:

Open-Vessel Microwave Digestion System

Automated 35-ton Hydraulic X-Press

Automated SPEX-Claissé 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

Evacuatable Pellet Dies and Spec-Caps

Graphite Crucibles for Fusions Nylon Sieve Sets

Shatterboxes, Mixer/Mills . . . AND MORE!

3rd EDITION

SPEX
HAND
BOOK
OF
SAMPLE
PREPARATION
AND
HANDLING

SPEX

INDUSTRIES, INC.
3880 PARK AVE. • EDISON, N.J. 08820
TEL: 908-549-7144 • FAX: 908-603-9647

Editor in Chief

Deane K. Smith
Department of Geosciences
The Pennsylvania State University
239 Deike Building
University Park, PA 16802-2711 U.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 Toraya
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, Czechoslovakia
V. A. Frank-Kamenetsky, Leningrad, U.S.S.R.
L. Frevel, Midland, Michigan
P. Gado, Budapest, Hungary
H. Goebel, Munchen, West Germany
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, MD
M. E. Mrose, Gaithersburg, MD
M. H. Mueller, Argonne, Illinois
M. Nichols, Livermore, California
B. Post, West Roxbury, Massachusetts
E. Prince, Gaithersburg, MD (IUCr Representative)
R. L. Snyder, Alfred, New York
S. Weissman, Piscataway, New Jersey
T. Yamanaka, Tokyo, Japan
R. A. Young, Atlanta, Georgia
L. Zevin, Beer-Sheva, Israel

AIP Production: Lin Miller, *Editorial Supervisor*;
Andrea Witt, *Journal Coordinator*;
Christine Joyce, *Senior Production Editor*

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.

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: AIP Advertising Department, 335 East 45th Street, New York, NY 10017-3483, (212) 661-9404 x361.

Subscription Prices (1993)

	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. 1993 single copies: \$30. Prior to 1993 single copies: \$30.

Subscription, renewals, and address changes should be addressed to *AIP Member and Subscriber Services*, 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 Member Services 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 0885-7156/93 \$06.00.

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 Member and Subscriber Services, 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. Application to mail at second class rates is pending at Woodbury, NY and additional mailing offices.

Copyright 1993 by JCPDS-International Centre for Diffraction Data.

Expand your x-ray diffraction capabilities — not your overhead.

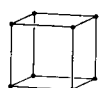
Whether you just need services or your XRD lab is on "overload," IC Laboratories provides every testing service and advanced capability you need in qualitative or quantitative x-ray diffraction analysis — from austenite to zeolites, from air filters to thin films. You are assured of rapid turn-around 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

We're the Specialists in XRD

For 1992/93 from ICDD...

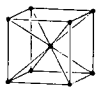


Set 42 PDF

In all current media

CD-ROM & Mag Tape... Microfiche ... Book

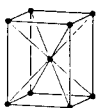
Over 2000 new &/or updated entries in PDF-1 and PDF-2†



EDD Electron Diffraction Data Base

(NIST/Sandia/ICDD)

Crystallographic & chemical data on over 71,000 crystalline materials.†



NIST Crystal Data File

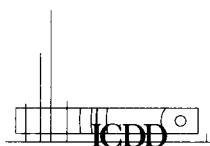
Crystallographic & chemical data on over 170,000 crystalline materials*

†Available for IBM-PC compatibles, VAX & Macintosh

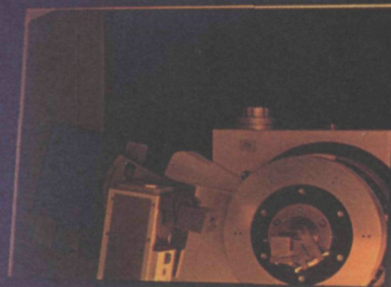
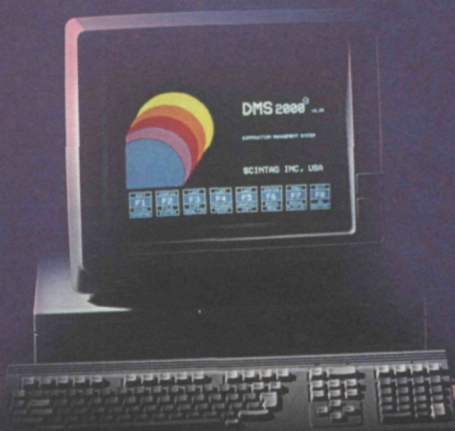
*Available for IBM-PC compatibles & VAX

International Centre for Diffraction Data

1601 Park Lane, Swarthmore, PA 19081 USA (215) 328-9400 Telex: 847170



We're Dedicated to Powder X-ray Diffraction



XDS

Powder X-ray diffraction is our specialty. In fact, it's all we do.

That's why we can deliver all those technological advances others only promise, including the largest selection of software in the industry. It's also why Scintag users enjoy the kind of after-the-sale support that helps them realize substantial returns on their investment, year after year. When it comes to powder X-ray diffraction technology, Scintag stands at the forefront with:

- **Highest resolution powder diffractometers**
- **Controlled-temperature XRD**
- **Controlled-atmosphere XRD**
- **Multi-user, multi-tasking operation**
- **Solid-state detectors**

So, for the latest innovations in powder diffraction, there's really only one choice: Scintag. But don't take our word for it. Contact us today for our full-color brochure and a complete system demonstration, and judge for yourself.



SCINTAG, Inc.

707 Kifer Road
Sunnyvale, CA 94086
Tel. (408) 737-7200
Fax (408) 737-9841

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



Fundamentals of X-ray Powder Diffraction— June 7-11, 1993:

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

Fundamentals of X-ray Fluorescence— June 21-25, 1993:

covering theoretical discussion of instrumentation for wavelength and energy dispersive spectrometry, specimen preparation, and simple quantitative methods.

Advanced Methods in Powder Diffraction— June 14-18, 1993:

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

Advanced Methods in X-ray Fluorescence— June 28-July 2, 1993:

with an emphasis on quantitative methods and use of automated X-ray spectrometers.



For further information contact: Theresa Maguire
1601 Park Lane, Swarthmore, Pennsylvania, 19081-2389, U.S.A.
Phone (215) 328-9400, FAX (215) 328-2503



International Centre for Diffraction Data

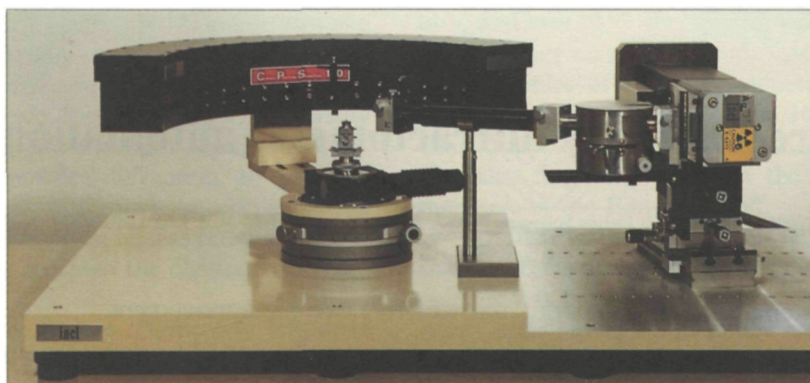
**X-ray
Diffraction
Reference Standards
and Zero-background
Sample Plates
Custom Designed
and Built for any
Application**

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.

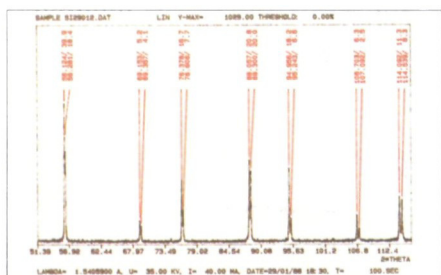
The Gem Dugout
1652 Princeton Drive
State College, PA 16803
(814) 865-5782

Powder Diffraction is published quarterly: March, June, September and December. Space reservations, insertion orders and materials are due February 1, May 1, August 1 and November 1. For more information and advertising rates, contact the advertising office at (212) 661-9260.

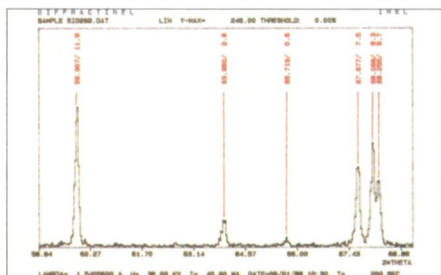
THE CHOICE OF THE FUTURE
SIMULTANEOUS XRD
OVER 120° - 2 THETA
- FAST - ACCURATE - RELIABLE -



CPS 120 MOUNTED ON TGS (TRANSMISSION AND REFLECTION MODE)



SILICON $\lambda = \text{CuK}\alpha$



QUARTZ Si O₂
 MONOCHROMATOR : QUARTZ



FAST DIFFRACTOMETER

ACCESSORIES :

**CRYOSTAT - FURNACE - SAMPLE SPINNER -
 AUTOMATIC SAMPLE CHANGER - and
 X-RAY GENERATOR etc...**

APPLICATIONS :

**POWDER, STRESS, and TEXTURE WITH
 MATCHING SOFTWARE**

inel

12, avenue de Scandinavie
 91953 LES ULIS CEDEX FRANCE
 PHONE 33 (1) 69.86.13.30
 FAX 33 (1) 69.86 14 19
 TELEX 603965

or: P.O. Box 147
 Stratham, NH 03885
 PHONE (603) 778-9161
 FAX (603) 778-9171


**ASK FOR MORE INFORMATION AND ADDRESS
 OF OUR REPRESENTATIVE IN YOUR COUNTRY**

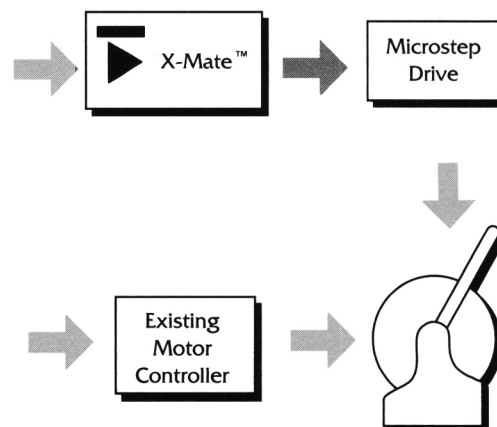
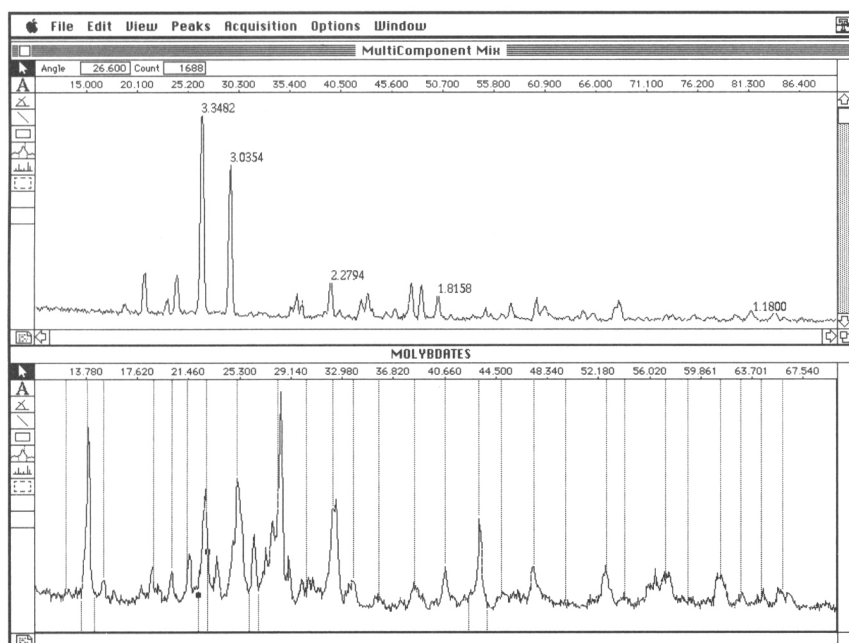
ThetaPlus[®]

Rebuild! Upgrade! Modernize!

A New Generation in X-ray Diffraction

Precise X-ray diffractometer automation:

- Search/Match incorporates  MacPDF[™] for JCPDS database CD-ROM access.
- X-Mate controller provides true background acquisition.
- Custom Microstep driver gives smooth, reproducible two-theta movement.
- Convenient user interface employs the enhanced graphics expected from the Macintosh II.



Is your present system automated but outdated?

ThetaPlus augments your diffractometer in two ways:

- **Upgrade** to our Microstep drive to increase two-theta resolution up to ten-fold without changing the existing stepping motor -OR-
- **Replace** only the outmoded computer and software by communicating directly with the existing motor controller.

We make your instruments perform!