49TH ANNUAL
DENVER X-RAY CONFERENCE

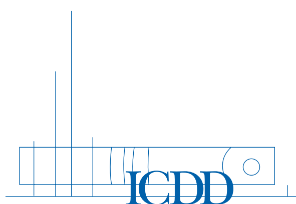
PROGRAM

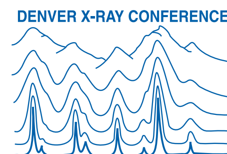
PLENARY SESSION

X-RAY ANALYSIS
in the
21ST CENTURY

31 JULY – 4 AUGUST 2000

DENVER MARRIOTT TECH CENTER HOTEL
DENVER, COLORADO U.S.A.





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INTERNATIONAL CENTRE FOR DIFFRACTION DATA

49th Annual Denver X-ray Conference

Denver Marriott Tech Center Hotel
Denver, Colorado U.S.A.
31 July – 4 August 2000

2000 Denver X-ray Conference Organizing Committee

Randolph Barton, Jr., DuPont Experimental Station, Wilmington, DE
Don Broton, Construction Technology Labs, Skokie, IL
Victor E. Buhrke, The Buhrke Company, Portola Valley, CA
John V. Gilfrich, SFA, Inc./NRL, Washington, DC
George J. Havrilla, co-Chair, Los Alamos National Laboratory, Los Alamos, NM
Ting C. Huang, Emeritus, IBM Almaden Research Center, San Jose, CA
Ron Jenkins, Chair, International Centre for Diffraction Data, Newtown Square, PA
Terry Maguire, Liaison, International Centre for Diffraction Data, Newtown Square, PA
I. Cev Noyan, IBM, Yorktown Heights, NY
Paul K. Predecki, Past Chair, University of Denver, Denver, CO
Deane K. Smith, Emeritus, The Pennsylvania State University, University Park, PA
Robert L. Snyder, The Ohio State University, Columbus, OH
Mary Ann Zaitz, IBM Microelectronics, Hopewell Junction, NY

Future Conference Dates:

30 July – 3 August 2001: Sheraton Steamboat Resort
Steamboat Springs, Colorado, U.S.A.

Program:

This program is also available on the Denver X-ray Conference web page at http://www.dxcicdd.com. The information contained in this program is current as of the printing date. Changes will be communicated at the conference.

2000 Denver X-ray Conference Program
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Accommodations and Travel

Hotel

The 2000 Denver X-ray Conference will be held 31 July – 4 August at the Denver Marriott Tech Center Hotel, 4900 S. Syracuse Street, Denver, CO 80237, U.S.A., phone: 1-800-228-9290 or dial direct: 1-303-779-1100, fax: 1-303-770-6112.

Reservations

Attendees are responsible for making their own reservations. Please identify yourself as a Denver X-ray Conference attendee when booking your reservation. Reservations should be made as soon as possible since there are a limited number of rooms available at the conference rate. The special conference rate of $104 per day (plus 11.8% tax) for single, double, triple or quadruple occupancy will only be applicable before 6 July 2000, subject to availability. Please note the hotel's cancellation policy: Individual room reservations may be canceled or changed until 6:00 p.m. on the scheduled date of arrival with no charge. Any reservations that are not cancelled (and the guest fails to arrive at the hotel) will be subject to a charge of one night's room and tax charge.

Students

A limited number of rooms are also available for students. Student rooms are $25 per bed, per day (plus 11.8% tax), two students per room. Please contact the Conference Coordinator, Denise Flaherty (flaherty@icdd.com), for detailed information regarding student rooms.

Travel Arrangements

The Denver X-ray Conference has selected Kitty Ward Travel, Inc. as the official travel agent for the conference. Kitty Ward Travel has negotiated special fares with United Airlines and US Airways. A request for air travel form is included on page 45 of this program. Please complete the form and fax to Kitty Ward Travel at fax: 610-543-0786 or call 610-543-0680 or 800-752-3718. If you prefer to arrange your own travel, you may still take advantage of the special airfares by referring to the Denver X-ray Conference numbers when making your reservations. The numbers are as follows:

United Airlines	Phone: 1-800-241-6522	DXC Reference Number: 596DS
US Airways	Phone: 1-800-428-4322	DXC Reference Number: 85181511

Registration Information

Conference Registration Fees*

All attendees must register for the conference, including organizers, chairs, invited speakers, and instructors.

*Discounted fees will be applied to registrations received before 14 July 2000. The reduced registration fee will only be applied if registration form and payment are received on or before 14 July 2000. Attendees may pre-register by completing the form on page 47 of this program and sending it to: Denise Flaherty, ICDD, 12 Campus Blvd., Newtown Square, PA 19073-3273, U.S.A. ◆ E-mail dxc@icdd.com ◆ phone 610-325-9814 ◆ fax 610-325-9823. Registration checks should be made payable to **ICDD/DXC** and enclosed with the registration forms.

	By July 14th	After July 14th
•Full week: exhibits, workshops, sessions†	$275	$325
•Monday & Tuesday: exhibits, workshops†	$225	$275
•Wednesday, Thursday & Friday: exhibits, sessions†	$225	$275
•Session organizers, invited speakers & workshop instructors†	$100	$100
•Students, unemployed X-ray people, and persons 65 and older: exhibits, workshops, sessions	$50	$50
•Conference dinner, Thursday evening	$30	$30

†Includes a copy of Volume 44 of ***Advances in X-ray Analysis*** on CD-ROM

Take advantage of this opportunity to include the following orders with your conference registration fee:

- ***Advances in X-ray Analysis,*** Cumulative Volumes 1–39 on CD-ROM: $350
- ***Advances in X-ray Analysis,*** Volume 40 on CD-ROM: $150
- ***Advances in X-ray Analysis,*** Volume 41 on CD-ROM: $150
- ***Advances in X-ray Analysis,*** Volume 42 on CD-ROM: $150
- ***Powder Diffraction***☆(Individual one year subscription for the year 2001): Domestic $60 / Overseas $85
- ***Powder Diffraction***☆(Institution one year subscription for the year 2001): Worldwide $105

☆***Powder Diffraction*** is a quarterly journal that focuses on materials characterization employing X-ray powder diffraction techniques and procedures. For more information, please call 1-516-576-2200.

On-site Registration:

All on-site registrations will be conducted at the Conference Registration Desk, located by the convention entrance on the ground floor (level one) of the Denver Marriott Tech Center Hotel.

AVOID LONG LINES! SAVE MONEY! PRE-REGISTER!

Registration Times:

Sunday, 30 July	4:00 p.m. – 7:00 p.m.
Monday, 31 July	7:30 a.m. – 3:00 p.m.
Tuesday, 1 August	8:00 a.m. – 3:00 p.m.
Wednesday, 2 August	8:00 a.m. – 2:00 p.m.
Thursday, 3 August	8:00 a.m. – 2:00 p.m.

Please Note: Attendees (even those pre-registered) should check-in at the Conference Registration Desk for conference materials (name tags, *Book of Abstracts*, late announcements, etc.).

Cancellation Policy: All cancellations will be assessed a $25 processing fee. Cancellations must be submitted in writing to the Conference Coordinator. A full refund will be issued, less processing fee, if the cancellation is received one week before the conference (Monday, 24 July 2000). No refunds will be issued for cancellations received after 24 July 2000.

Exhibitor Information

Exhibits will be located in the Columbine Center on the ground floor (level one) of the hotel. A diagram of the exhibit locations will be available in the *Book of Abstracts*.

Exhibit Hours:

Monday	10:00 a.m. to 5:00 p.m.
Tuesday	10:00 a.m. to 5:00 p.m.
Wednesday	10:00 a.m. to 5:00 p.m.
Thursday	10:00 a.m. to 2:00 p.m.

Exhibitors as of 1 May 2000

AMPTEK, Inc.

Angstrom, Inc.

ARL/Scintag

ATPS, Inc. (Advanced Technical Products & Services)

Bede Scientific Incorporated

Bertan High Voltage/Del Electronics

Blake Industries, Inc.

Bruker AXS, Inc.

Chemplex Industries, Inc.

Diffraction Technology/Rocklabs

EDAX, Inc.

Gresham Scientific Instruments

ICPH Chemical International/Socachim

INEL

International Centre for Diffraction Data (ICDD)

ITAL STRUCTURES

Jordan Valley AR, Inc.

KevexSpectrace

Kratos Analytical, Inc.

K-TEK International, Inc.

LND, Inc.

Materials Data, Inc. (MDI)

MOXTEK, Inc.

Osmic, Inc.

Philips Analytical

Premier Lab Supply

Rigaku/USA, Inc.

Spectro Analytical Instruments

SPEX CertiPrep, Inc.

X-ray Optical Systems, Inc.

All exhibitors are invited to attend the

Exhibitors' General Meeting

Wednesday, 2 August 2000, 6:00 – 6:30 p.m. in the **Conifer 2 Room**

Evening Technical Sessions and Social Functions

—Spouses are welcome to attend all social functions
—Evening Mixers and Poster Sessions will be held in the ***Evergreen Ballroom*** unless otherwise noted

Sun., 30 July	5:30 – 7:30	Welcoming Reception (to be held in the **Atrium**) Sponsored by Bede Scientific, SPEX CertiPrep and Claisse Scientifique
Mon., 31 July	6:30 – 8:30	Philips Analytical Reception & XRD Poster Session I Sponsored by Philips Analytical, Inc.
Tues., 1 August	6:30 – 8:30	MDI and Rigaku/USA Reception & XRD Poster Session II Sponsored by Materials Data, Inc. and Rigaku/USA
Wed., 2 August	6:30 – 8:30	Bruker AXS, Inc. Reception & XRF Poster Session Sponsored by Bruker AXS, Inc.
Thurs., 3 August	7:00	Conference Dinner Tickets will be sold at the conference registration desk, located by the convention entrance on the ground floor (level one) of the Denver Marriott Tech Center Hotel, until Wednesday at noon. Cost: $30 per ticket. After dinner, Deane Smith will present a lecture entitled "Gems: The Usual and Unusual".

Spouses' Coffee Hour:

All spouses are invited to attend a complimentary coffee hour, sponsored by the Denver X-ray Conference. Coffee, tea and pastries will be served in the **Conifer 2 Room** from 9:30 to 10:30 a.m. on Monday through Wednesday. Information on local attractions and activities of interest will be provided.

General Information:

ICDD Meetings:

A schedule of ICDD task group meetings will be posted at the conference.

Employment Clearinghouse:

We will have a separate bulletin board to announce employment opportunities. Prospective employers and employees should bring announcements with them for posting.

Book of Abstracts:

Available at the conference registration desk.

Workshops
Monday, 31 July – Tuesday, 1 August
a.m. workshops: 9:00 a.m. – 12:00 noon p.m. workshops: 2:00 p.m. – 5:00 p.m.
Unless otherwise noted:

Workshops, Monday a.m.

XRD & XRF

W-1 New Methods of Beam Conditioning (Evergreen A)

Organizer: **J. Faber,** International Centre for Diffraction Data, Newtown Square, PA

Instructors: **J. Faber,** International Centre for Diffraction Data, Newtown Square, PA
D.K. Bowen, Bede Scientific, Inc., Englewood, CO

This workshop discusses traditional and newer methods of X-ray beam conditioning, as applied to both X-ray diffraction and X-ray fluorescence.

XRD

W-2 Hands on Rietveld Analysis I (Bring your own computer) (Evergreen B)

Organized by: **R.E. Dinnebier,** University of Bayreuth, Bayreuth, Germany
E. Antipov, Moscow State University, Moscow, Russia

Instructors: **R.E. Dinnebier,** University of Bayreuth, Bayreuth, Germany
E. Antipov, Moscow State University, Moscow, Russia
R. VonDreele, Los Alamos National Laboratory, Los Alamos, New Mexico
P.W. Stephens, State University of New York at Stony Brook, Stony Brook, NY

The Rietveld method is a fast-developing technique. This course is intended for beginners as well as advanced users and will cover many new features such as: advanced peak profile functions, rigid bodies with satellite groups, planarity restraints, modeling of anisotropic half-widths due to lattice strain, etc. After the lectures, all participants will have the opportunity to practice* using the well known "GSAS" program system. A well-prepared example exhibiting different levels of complexity will be provided. Participants are also welcome to bring their own datasets.

*In order to participate hands-on, you must bring your own laptop computer and load the appropriate software, prior to attending the workshop. Please visit the web page http://www.pulverdiffraktometrie.de/Education/rietveld/rietveld.html for detailed instructions on how to obtain the necessary software.

W-3 Alignment & Standards (Evergreen C)

Organizers & Instructors: **J.P. Cline,** National Institute of Standards & Technology, Gaithersburg, MD
R.W. Cheary, University of Technology Sydney, New South Wales, Australia

This workshop will discuss NIST Standard Reference Materials, the basic design of the conventional diffractometer, and how to realize optimal diffractometer performance through proper alignment and selection of optical components (eg., divergence slits, Soller slits, etc.). Various alignment procedures will be discussed with consideration given to the consequences of misalignment and missetting of the components. Instrument calibration and performance will be evaluated through the use of NIST Standards and the simulation of line profiles.

XRF

W-4 Practical TXRF (Evergreen D)

Organized by: **M.A. Zaitz,** IBM Microelectronics, Hopewell Junction, NY

Instructors: **M.A. Zaitz,** IBM Microelectronics, Hopewell Junction, NY
P. Wobrauschek, Atominstitut der Österreichischen Universitäten, Vienna, Austria
C. Streli, Atominstitut der Österreichischen Universitäten, Vienna, Austria

This workshop will cover the basics of total reflection X-ray fluorescence, as well as instrumentation, calibration, and applications.

Workshops, Monday p.m.

XRD

W-5 Hands on Rietveld Analysis II (Bring your own computer) (Evergreen B)

Organized by: **R.E. Dinnebier,** University of Bayreuth, Bayreuth, Germany
E. Antipov, Moscow State University, Moscow, Russia

Instructors: **R.E. Dinnebier,** University of Bayreuth, Bayreuth, Germany
E. Antipov, Moscow State University, Moscow, Russia
R. VonDreele, Los Alamos National Laboratory, Los Alamos, New Mexico
P.W. Stephens, State University of New York at Stony Brook, Stony Brook, NY

Continuation of W-2.

*In order to participate hands-on, you must bring your own laptop computer and load the appropriate software, prior to attending the workshop. Please visit the web page http://www.pulverdiffraktometrie.de/Education/rietveld/rietveld.html for detailed instructions on how to obtain the necessary software.

W-6 Analysis of Micron Size Specimens (Evergreen A)

Organized by: **R. Goehner,** Sandia National Laboratories, Albuquerque, NM

Instructors: **R. Goehner,** Sandia National Laboratories, Albuquerque, NM
R. Tissot, Sandia National Laboratories, Albuquerque, NM
G. Ice, Oak Ridge National Laboratory, Oak Ridge, TN
P.-C. Wang, IBM Corporation Microelectronics Division, Hopewell Junction, NY

The workshop will describe methods and techniques used to analyze micron size specimens. Instructors will cover such topics as the use of Scanning Electron Microscopy for crystallographic evaluation, synchrotron based X-ray microbeam characterization of thin films in very-large-scale-integrated circuits, recent advances in synchrotron based 3-D X-ray crystal microscopes, and the use of laboratory-based X-ray sources and 2-D area detectors for small specimen analysis. Please bring your questions and ideas to this open forum workshop.

XRF

W-7 An Introduction to X-ray Fluorescence (Evergreen C)

Organized by: **R. Jenkins,** International Centre for Diffraction Data, Newtown Square, PA

Instructors: **R. Jenkins,** International Centre for Diffraction Data, Newtown Square, PA
J. Croke, Philips Analytical, Inc. (retired), Mahwah, NJ

This workshop is intended for beginners and those fairly new to the field of X-ray fluorescence analysis. The principles behind the technique, along with a description of the basics, of X-ray spectra and absorption effects will be introduced. The various types of instrumentation used in the field, including a "compare and contrast" of the features of wavelength and energy dispersive spectrometers, will also be presented. The use of both techniques for qualitative analysis will be covered. Additionally, brief coverage on specimen preparation methods an introduction to the basic concepts behind quantitative analysis will be offered.

W-8 Analysis of Layered Materials by XRF (Evergreen D)

Organized by: **M.W. Dirken,** Philips Analytical, Almelo, The Netherlands

Instructors: **M.W. Dirken,** Philips Analytical, Almelo, The Netherlands
M. Mantler, Vienna University of Technology, Vienna, Austria
A. Wittkopp, Rontgenanalytik, Taunusstein-Neuhof, Germany

This workshop provides an introduction to the analysis of layered materials, and is intended for the X-ray spectroscopist who encounters this analysis for the first time. Therefore, the physics and various analysis models are presented. This is followed by contributions on ED-XRF and WD-XRF examples, focusing on practical issues including problems of finite thickness and line selection.

Workshops, Tuesday a.m.

XRD

W-9 Residual Stress Analysis (Evergreen A)

Organized by: **I. C. Noyan,** IBM Research Division, Yorktown Heights, NY
C.C. Goldsmith, IBM Microelectronics, Hopewell Junction, NY

Instructors: **I. C. Noyan,** IBM Research Division, Yorktown Heights, NY
C.C. Goldsmith, IBM Microelectronics, Hopewell Junction, NY
T. Nunes, IBM Microelectronics (retired), Hopewell Junction, NY

This workshop will cover the basic theory of diffraction stress analysis and its application to real problems. Those who attend should be able to evaluate a result to see if it is consistent with applicable theory.

W-10 Phase Transformation (Evergreen B)

Organized by: **H. Jones,** Pratt & Whitney, East Hartford, CT

Instructors: **H. Jones,** Pratt & Whitney, East Hartford, CT
A. Voskamp, SKF Engineering and Research Centre B.V., DT Nieuwegein, The Netherlands
R. England, Cummins Engine Company, Columbus, IN

This workshop will review specific and general applications of X-ray diffraction to the study of phase transformations in metals. Specific applications will be the evaluation of retained austenite in heat treated steels before and after use and sample preparation methods to isolate phases for phase transformation studies in nickel superalloys. Wavelength and energy dispersive methods, sample preparation, stability of X-ray tubes, and examples of phase transformations in metal processing will be discussed. Crystal chemistry and use of ICDD products will also be included.

XRF

W-11 Specimen Preparation – XRF I (8:30 a.m. – 12:00 noon) (Evergreen C)

Organized by: **V. Buhrke,** The Buhrke Company, Portola Valley, CA

Instructors: **J. Willis,** James Willis Consultants, Somerset West, South Africa
D. Broton, Construction Technology Laboratories, Inc., Skokie, IL
R. Bostwick, SPEX CertiPrep, Inc., Metuchen, NJ
B. Wheeler, Rigaku/USA, Inc. (retired), Danvers, MA
L. Creasy, TIMET, Morgantown, PA

This full day workshop will cover sample preparation of geological materials; fused bead preparation in the cement industry; cement kiln feed, raw materials and alternate raw materials; pitfalls in the use of sample preparation equipment; the preparation of liquid, small, and irregular shaped specimens; and the preparation of metal specimens for XRF analysis. A question and answer period will follow.

Workshops, Tuesday a.m.

W-12 Fundamental Parameters (Evergreen D)

Organized by: **M. Mantler,** Vienna University of Technology, Vienna, Austria

Instructors: **M. Mantler,** Vienna University of Technology, Vienna, Austria
B. Vrebos, Philips Analytical, Almelo, The Netherlands
W.T. Elam, Naval Research Laboratory, Washington, DC

This workshop will cover:

- Atomic ("fundamental") parameters and tube spectra: Definitions, sources (tables, available data files, computed data and related algorithms), accuracy
- Theoretical background: Physical-mathematical models for primary and secondary excitation, Coster-Kronig transitions; Conventional equations and Monte-Carlo methods
- Software issues: Technical aspects, availability
- Fundamental parameters and computed influence coefficients
- Thin films, inhomogeneous specimens, light elements
- Practical applications

On-line support by (noncommercial) fundamental parameter software will be available.

Workshops Tuesday p.m.

XRD

W-13 Grazing Incidence (Evergreen B)

Organizer & Instructor: **T.C. Huang,** Emeritus, IBM Almaden Research Center, San Jose, CA

co-Chair: **J. Harada,** Rigaku Corporation, Tokyo, Japan

This workshop covers the theoretical background, experimental methods and applications of grazing-incidence X-rays for the characterization of surfaces and thin films. Three commonly used grazing-incidence techniques are: the in-plane diffraction, asymmetric Bragg diffraction, and reflectivity. Technical details and the applications of these techniques for characterizing high-tech materials (e.g., high-density magnetic recording media, two-dimensional monolayer, Mo/Si multilayers, etc.) will be given.

W-14 Texture Analysis (1:30 p.m. – 6:30 p.m.) (Evergreen D)

Organized by: **R. De Angelis,** Visiting Professor, University of Florida, Shalimar, FL
H. Schaeben, Freiberg University of Technology and Mining, Freiberg, Germany

Instructors: **R. De Angelis,** Visiting Professor, University of Florida, Shalimar, FL
T. Snyder, Union Pacific Railroad, Omaha, NE
H. Schaeben, Freiberg University of Technology and Mining, Freiberg, Germany

This workshop covers the application of texture analysis and some of the pitfalls and difficulties encountered. Topics include: X-ray optics in texture determination from flat and slightly curved specimens; how background and defocusing corrections are handled in data analysis in determination of the integrated intensities; intensity data processing to pole figures, inverse pole figures and ODFs using popLA; textures of deformed copper and tantalum and of tapered steel roller bearings; determining fractions of major crystallographic poles texture data along fibers in ODF space. Evaluation of texture goniometer data with the results of scanning the spherical X-ray transform of an orientation density function is considered. A unifying view of texture analysis is presented as applied to spherical tomography.

XRF

W-15 Specimen Preparation – XRF II (1:00 p.m. – 4:45 p.m.) (Evergreen C)

Organized by: **V. Buhrke,** The Buhrke Company, Portola Valley, CA

Instructors: **J. Willis,** James Willis Consultants, Somerset West, South Africa
D. Broton, Construction Technology Laboratories, Inc., Skokie, IL
R. Bostwick, SPEX CertiPrep, Inc., Metuchen, NJ
B. Wheeler, Rigaku/USA, Inc. (retired), Danvers, MA
L. Creasy, TIMET, Morgantown, PA

Continuation of W-11.

W-16 Quantitative Analysis – Standardless Methods (Evergreen A)

Organized by: **J.A. Anzelmo,** Bruker AXS, Inc., Madison, WI

Instructors: **J.A. Anzelmo,** Bruker AXS, Inc., Madison, WI
K.M. Mauser, Bruker AXS GmbH, Karlsruhe, Germany
R. Yellepeddi, ARL, Ecublens, Switzerland

Two approaches have emerged as the methods of performing so-called Standardless Analysis. The two approaches are 1) scanning, and 2) counting directly on peaks and backgrounds. This workshop will discuss various aspects of the two approaches such as the theory, data collection, data manipulation, calibration, sample preparation, and practical examples.

Sessions
Poster Sessions: Monday, 31 July – Wednesday, 2 August
Oral Sessions: Wednesday, 2 August – Friday, 4 August

XRD Poster Session I, Monday, 31 July (Evergreen Ballroom)

(6:30 p.m. – 8:30 p.m., authors present)

The XRD Poster Session will be held in conjunction with the Philips Analytical mixer.

Chairs: **T.C. Huang,** Emeritus, IBM Almaden Research Center, San Jose, CA
R.L. Snyder, The Ohio State University, Columbus, OH

Session chairs will select the two best papers for awards.

ICDD Grant-in-Aid Program, Standard Reference Materials

D-001 ICDD GRANT-IN-AID PROGRAM

T. Kahmer, R. Jenkins, International Centre for Diffraction Data, Newtown Square, PA

D-082 STANDARD REFERENCE MATERIAL (SRM 1990) FOR SINGLE CRYSTAL DIFFRACTOMETER ALIGNMENT

W. Wong-Ng, J. Armstrong, M. Levenson, L.P. Cook, National Institute of Standards and Technology, Gaithersburg, MD
T. Siegrist, Lund University, Sweden
G. DeTitta, Hauptman-Woodward Medical Research Institute, Buffalo, NY
L. Finger, Geophysical Laboratory, Washington, DC
H. Evans, U.S. Geological Survey, Reston, VA
E. Gabe, G. Enright, SIMS, Ottawa, Canada
C.R. Hubbard, Oak Ridge National Laboratory, Oak Ridge, TN

Structure Investigations

D-024 NEUTRON VERIFICATION OF X-RAY DERIVED THERMAL PARAMETERS IN Ni SUBSTITUTED CuAu I ALLOYS

R. Kumar, East Carolina University, Greenville, NC
W.B. Yelon, University of Missouri Research Reactor

D-015 PREDICTION OF THE CRYSTAL STRUCTURE OF BINARY AND TERNARY INORGANIC COMPOUNDS USING SYMMETRY RESTRICTIONS AND POWDER DIFFRACTION DATA

L. Reinaudi, P. Serra, E.P.M. Leiva, R.E. Carbonio, Universidad Nacional de Córdoba, Córdoba, Argentina

D-010 A CONTINUOUS ELECTRON DENSITY APPROACH IN RIETVELD ANALYSIS FOR STRUCTURE INVESTIGATIONS OF THE MESOPOROUS SILICATE MATERIALS

L.A. Solovyov, S.D. Kirik, Institute of Chemistry and Chemical Engineering, Krasnoyarsk, Russia
A.N. Shmakov, V.N. Romannikov, Boreskov Institute of Catalysis, Novosibirsk, Russia

D-009 MESOPOROS SILICATE MATERIALS: LOOK INSIDE WITH HELP OF X-RAY DIFFRACTION

S.D. Kirik, L.A. Solovyov, Institute of Chemistry and Chemical Engineering, Krasnoyarsk, Russia
V.N. Romannikov, A.N. Shmakov, Boreskov Institute of Catalysis, Novosibirsk, Russia

D-008 IN SITU X-RAY DIFFRACTION STUDIES OF YbCo THICK FILM CRYSTALLIZATION

A. Puig-Molina, H. Graafsma, European Synchrotron Radiation Facility, ESRF, Grenoble, France
T. Puig, S. Piñol, X. Obradors, Institut de Ciencia de Materials de Barcelona, Bellaterra, Spain

D-032 CHARACTERISTICS OF THE CRYSTAL STRUCTURE AND MICROSTRUCTURE OF THE $MgNb_2O_6$ and $PbMg_{1/3}Nb_{2/3}O_3$ PREPARED VIA CHEMICAL ROUTES

C.O. Paiva-Santos, A.A. Cavalheiro, M.A. Zaghete, M. Cilense, J.A. Varela, UNESP.Araraquara, SP Brazil
M.T. Silva Giotto, UFSCar. São Carlos, SP Brazil
Y.P. Mascarenhas, USP. São Carlos, SP Brazil

D-056 X-RAY MICRODIFFRACTION ON A SMALL PIECE OF SKIN OF THE WORLD-FAMOUS “OETZI” (TYROLEAN MUMMIFIED GLACIERMAN) BY USING THE D8 DISCOVER WITH GADDS

J. Brechbuehl, A. Kern, H. Jakob, Bruker AXS GmbH, Karlsruhe, Germany
R. Tessadri, University of Innsbruck, Innsbruck, Austria

C-3 QUANTIFICATION OF CLINKER AND CEMENT PHASES WITH THE HIGHEST SPEED AND ACCURACY USING XRD

A. Kern, Bruker AXS GmbH, Karlsruhe, Germany

D-123 CRYSTAL STRUCTURE OF A NEW POLYMORPH OF SULFABENZAMIDE

J.A. Kaduk, BP Amoco p.l.c., Naperville, IL
S.J. Maginn, J. Cole, Cambridge Crystallographic Data Centre, Cambridge, United Kingdom
K.M. Shankland, CLRC Rutherford Appleton Laboratory, Oxon, United Kingdom

XRD Instrumentation, Texture

D-002 NON-TRADITIONAL EQUIPMENT FOR THE MEASUREMENT OF POWDER PATTERNS

J. Faber, G. Grosse, S. Kabekkodu, R. Jenkins, International Centre for Diffraction Data, Newtown Square, PA

D-003 TRADITIONAL EQUIPMENT FOR THE MEASUREMENT OF POWDER PATTERNS

R. Jenkins, International Centre for Diffraction Data, Newtown Square, PA

D-085 SHUTTER FAILURE RADIATION MONITOR SAFETY SYSTEM

C.R. Hubbard, T.R. Watkins, G.K. Schulze, Oak Ridge National Laboratory, Oak Ridge, TN

D-022 ANGLE MEASURING DEVICE FOR X-RAY COMPORATOR

I.A. Brytov, G.D. Dmitriev, V.N. Ivanov, Bourevestnik, Inc., St. Petersburg, Russia

D-066 COMPLETE POLE FIGURE MEASUREMENT BY ONLY BACK REFLECTION METHOD USING IMAGING PLATE AND APPLICATION TO THREE DIMENSIONAL ANALYSIS OF TEXTURE

T. Goto, T. Kondoh, Aichi Institute of Technology, Toyota, Japan
H. Hirose, Kinjyo College, Mattou, Japan
T. Sasaki, Kanazawa University, Kanazawa, Japan

D-096 QUANTITATIVE TEXTURE ANALYSIS WITH AN AREA DETECTOR

K.J. Kozaczek, R.I. Martin, P.R. Moran, D.S. Kurtz, HyperNex, Inc., State College, PA

High-Temperature and Non-Ambient Applications

D-083 PHASE TRANSITION AND DEHYDRATION BEHAVIOR OF ALPHA, ALPHA-TREHALOSE DIHYDRATE MEASURED BY XRD-DSC

S. Munekawa, A. Kishi, M. Shiro, Rigaku Corporation, Tokyo, Japan

D-049 HIGH TEMPERATURE X-RAY DIFFRACTION STUDIES OF PHASE FORMATION IN PORCELAINS

D.I. Seymour, W.M. Carty, S.T. Misture, New York State College of Ceramics at Alfred University, Alfred, NY

D-048 USING RELATIVE THERMAL EXPANSION AS A TEMPERATURE CALIBRATION METHOD FOR HTXRD

A.R. Drews, Ford Research Laboratories, Dearborn, MI

D-126 HIGH TEMPERATURE POWDER DIFFRACTION STUDY OF PHASE TRANSFORMATIONS IN THE BISMUTH CALCIUM OXIDE SYSTEM

A. Payzant, S. Nunn, W. Porter, R. Peascoe, Oak Ridge National Laboratory, Oak Ridge, TN

Applications, Miscellaneous

D-036 CHARACTERIZATION OF A COMBINATORIAL EPITAXIAL THIN-FILM LIBRARY USING A CONVERGENT-BEAM X-RAY DIFFRACTION SYSTEM

T. Kikuchi, K. Omote, J. Harada, Rigaku Corporation, Tokyo, Japan
M. Kawasaki, A. Ohtomo, M. Ohtani, T. Ohnishi, D. Komiyama, H. Koinuma, Tokyo Institute of Technology, Yokohama, Japan

D-098 RIETVELD ANALYSIS IN QUANTIFICATION OF METASTABLE POLYMORPHS OF ALUMINA

M. Shumsky, D. Winter, Rigaku/USA, Inc., The Woodlands, TX

D-124 ADVENTURES IN CORROSION DEPOSITS

J.A. Kaduk, BP Amoco p.l.c., Naperville, IL

D-120 ACTIVITIES OF THE ICDD EDUCATION SUBCOMMITTEE

S. Quick, Chair of the ICDD Education Subcommittee, The Pennsylvania State University, University Park, PA

D-121 ICDD ACTIVITY IN RUSSIA

E. Antipov, ICDD Regional co-Chair, Moscow State University, Moscow, Russia

D-122 POLYMER DIFFRACTION AT ICDD

S. Murthy, Chair of the ICDD Polymer Subcommittee, Allied Signal, Inc., Morristown, NJ

XRD Poster Session II, Tuesday, 1 August (Evergreen Ballroom)

6:30 p.m. – 8:30 p.m., authors present

The XRD Poster Session II will be held in conjunction with the MDI and Rigaku/USA mixer.

Chairs: **B.H. O'Connor,** Curtin University of Technology, Perth, Australia
P.K. Predecki, The University of Denver, Denver, CO

Session chairs will select the two best papers for awards.

TUESDAY XRD POSTER SESSION

Strain and Stress Analysis

D-064 FUNDAMENTAL EXPERIMENT ON NEUTRON STRESS MEASUREMENT USING NEUTRON IMAGE PLATE

T. Sasaki, Y. Hirose, Kanazawa University, Kanazawa, Japan
N. Minakawa, Y. Morii, N. Niimura, Japan Atomic Energy Research Institute, Ibaraki-ken, Japan

D-033 THE DEVELOPMENT OF MEASUREMENT TECHNIQUE FOR THE UNSTRESSED VALUE BY NEUTRON DIFFRACTION METHOD

N. Minakawa, Y. Morii, Japan Atomic Energy Research Institute, Ibaraki, Japan
T. Saito, T. Sasaki, Y. Hirose, Kanazawa University, Kanazawa, Japan

D-034 NON-DESTRUCTIVE MEASUREMENT OF RESIDUAL STRESS VERSUS DEPTH USING SYNCHROTRON RADIATION

R.D. England, Cummins Engine Company, Columbus, IN
T.R. Watkins, Oak Ridge National Laboratory, Oak Ridge, TN
N. Jayaraman, University of Cincinnati, Cincinnati, OH

D-042 ANALYSIS OF RESIDUAL STRESS STATE IN SPEED GEARS FOR AUTOMOTIVE VEHICLES

T. Gurova, J.R. Teodósio, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brasil
V. Monine, Instituto Politécnico do Rio de Janeiro, Nova Friburgo, Brasil

D-021 MICROSTRAIN ANALYSIS WITH SUB-μm DEPTH RESOLUTION IN SURFACE NITRIDED STAINLESS STEEL

S. Grigull, Å. Kvick, European Synchrotron Radiation Facility, Grenoble, France
S. Parascandola, Institut für Ionenstrahlphysik und Materialforschung, Dresden, Germany

D-062 STUDY ON EVALUATION OF RESIDUAL PHASE STRESS OF THE DUAL PHASE STAINLESS STEEL

H. Hirose, Kinjo Junior College, Matto, Japan
H. Hashi, T. Sasaki, Kanazawa University, Kanazawa, Japan

D-063 STUDY ON FRACTURE ANALYSIS OF $(\alpha + \beta)$ DUAL PHASE STAINLESS STEEL USING X-RAY DIFFRACTION

H. Hirose, Kinjo Junior College, Matto, Japan
T. Hamagami, T. Sasaki, Kanazawa University, Kanazawa, Japan

D-069 EFFECT OF X-RAY RESIDUAL STRESS IN SHOT-PEENED STAINLESS STEELS

S. Takahashi, T. Murotani, Y. Hirose, Kanazawa University, Kanazawa, Japan
M. Hashimoto, Sumitomo Heavy Industries, LTD., Aichi, Japan

D-060 A NEUTRON DIFFRACTION STUDY OF RESIDUAL STRAINS IN TWO MMC SYSTEMS; Ti/SiC AND W/Fe

P. Rangaswamy, H. Choo, M.A.M. Bourke, Los Alamos National Laboratory, Los Alamos, NM
A. Saigal, Tufts University, Medford, MA

D-068 MEASUREMENT OF RESIDUAL PHASE STRESS OF THE METAL MATRIX COMPOSITE MATERIAL USING SYNCHROTRON RADIATION

S. Takago, T. Sasaki, Y. Hirose, Kanazawa University, Kanazawa, Japan
K. Akita, Tokyo Metropolitan University, Tokyo, Japan
Y. Yoshioka, Musashi Institute of Technology, Tokyo, Japan

D-071 FABRICATION AND EVALUATION OF RESIDUAL STRESS FOR DISKSHAPED SYMMETRIC FUNCTIONALLY GRADED MATERIALS OF Ni/Al_2O_3 SYSTEM

K. Kikuchi, Y.-S. Kang, A. Kawasaki, Tohoku University, Sendai, Japan
T. Sasaki, Kanazawa University, Kanazawa, Japan

D-065 X-RAY STRESS DETERMINATION OF COLD-ROLLED STEEL SHEET USING ORIENTATION DISTRIBUTION FUNCTION

S. Ejiri, Y. Shirasuna, Seisen Jogakuin College, Nagano, Japan
T. Sasaki, Y. Hirose, Kanazawa University, Kanazawa, Japan
H. Inoue, University of Osaka Prefecture, Osaka, Japan

D-067 COMPOSITION DEPENDENCE OF X-RAY ELASTIC CONSTANT OF TITANIUM ALUMINIDE INTERMETALLIC COMPOUND

T. Kondoh, T. Goto, Aichi Institute of Technology, Toyota, Japan
T. Sasaki, Y. Hirose, Kanazawa University, Kanazawa, Japan

D-070 X-RAY ELASTIC CONSTANTS AND MECHANICAL ELASTIC CONSTANTS OF POLYCRYSTALLINE MATERIALS WITH ARBITRARY CRYSTAL STRUCTURES

Z. Lin, J. He, T. Sasaki, Y. Hirose, Kanazawa University, Kanazawa, Japan

X-ray Reflectometry

D-076 APPLICATION OF GIXR TO SOME INDUSTRIAL MATERIALS

H.J. Holland, Corning Inc., Corning, NY

D-023 THE USE OF X-RAY REFLECTOMETRY FOR SINGLE FILM THICKNESS ANALYSIS IN GMR MULTILAYER STACKS

C. Schug, B. York, J. Marien, H.-R. Blank, IBM Storage Technology Division

6:30 p.m. – 8:30 p.m., authors present

The XRF Poster Session will be held in conjunction with the Bruker AXS, Inc. mixer.

Chairs: **R. van Grieken,** University of Antwerp, Antwerp, Belgium
G. Havrilla, Los Alamos National Laboratory, Los Alamos, NM

Session chairs will select the three best papers for awards.

XRF Applications

F-25 INVESTIGATION OF THE TXRF DETECTION SENSITIVITY FOR LOW Z ELEMENTS AT THE PTB MONOCHROMATOR BEAMLINE FOR UNDULATOR RADIATION AT BESSY II

B. Beckhoff, G. Ulm, Physikalisch-Technische Bundesanstalt, Berlin, Germany
C. Streli, P. Wobrauschek, Atominstitut der Österreicheschen Universitäten, Wien, Austria
L. Fabry, S. Pahlke, Wacker Siltronic AG, Burghausen, Germany

F-53 THE USE OF XRF TO CONTROL A LANTHANIDE BENEFICIATION PLANT

E.B. McNew, Molycorp, Inc., Mt. Pass, CA
J. Willis, James Willis Consultants cc, Somerset West, South Africa

F-12 ANALYSIS OF THE PIGMENTS USED IN THE SCROLL PAINTINGS OF THE TALE OF GENJI, NATIONAL TREASURE, BY PORTABLE X-RAY FLUORESCENCE SPECTROMETER

K. Sugihara, K. Tamuara, M. Satoh, Seiko Instruments, Inc., Chiba, Japan
Y. Hayakawa, Y. Hirao, S. Miura, Tokyo National Research Institute of Cultural Properties, Tokyo, Japan
H. Yotsutsuji, Y. Tokugawa, Tokugawa Art Museum, Aichi, Japan

F-01 X-RAY FLUORESCENCE ANALYSIS BASED ON KNOWLEDGE SYSTEM

L. Luo, X. Wu, L. Gan, G. Liang, G. Ma, National Research Center of Geoanalysis, Beijing, China

F-50 COMPARISON OF TXRF ANALYSIS AND EDXRF WITH 150 nm AP1 SAMPLE SUPPORT FILMS

P. Wobrauschek, G. Buzanich, N. Marosi, Atominstitut der Österreichischen Universitäten, Vienna, Austria

XRF Instrumentation

F-26 THE BAM BEAMLINE AT THE ELECTRON STORAGE RING BESSY II – A SUITABLE SOURCE FOR X-RAY FLUORESCENCE ANALYSIS

B. Beckhoff, R. Klein, M. Krumrey, G. Ulm, Physikalisch-Technische Bundesanstalt, Berlin, Germany
W. Görner, B.R. Müller, H. Riesemeier, Bundesanstalt für Materialforschung und-prüfung, Berlin, Germany

F-31 ID18F, A NEW END-STATION AT THE ESRF FOR QUANTITATIVE μ-XRF ANALYSIS: PRELIMINARY EXPERIMENTS

B. Vekemans, A. Somogyi, L. Vincze, K. Janssens, F. Adams, University of Antwerp, Wilrijk, Belgium
M. Drakopoulos, A. Snigirev, ESRF, Grenoble, France

F-18 INTERACTIVE SOFTWARE FOR UPLOADING PROCESSED X-RAY FLUORESCENCE DATA FILES TO A LABORATORY INFORMATION MANAGEMENT SYSTEM (LIMS)

J.R. Quagliano, C.G. Worley, Los Alamos National Laboratory, Los Alamos, NM

F-46 X-RAY FLUORESCENCE ANALYSIS OF LOW-Z ELEMENTS INDUCED BY A FEMTOSECOND LASER

C. Streli, P. Wobrauschek, Atominstitut der Österreichischen Universitäten, Vienna, Austria
M. Schnürer, M. Hentschel, R. Kienberger, Ch. Spielmann, F. Krausz, Technische Universität Wien, Austria

F-33 SPECTRUM MODIFICATION IN THE X-RAY BEAM PASSED THROUGH A SLITLESS COLLIMATOR

V.K. Egorov, A.P. Zuev, IPTM RAS, Moscow District, Russia
E.V. Egorov, Moscow Engineering and Physical Institute, Moscow, Russia

F-07 HPGe DETECTOR RESPONSE FUNCTION TO LOW-ENERGY X-RAYS

M.C. Lépy, S. Forget, L. Loubet, J. Plagnard, Laboratoire National Henri Becquerel, France
C. Rémond, P. Stemmler, CEA/DAM, France

F-54 USING A CHARGE-COUPLED DEVICE (CCD) TO GATHER X-RAY FLUORESCENCE (XRF) AND X-RAY DIFFRACTION (XRD) INFORMATION SIMULTANEOUSLY

A. Reyes, H.K. Pew, P. Moody, MOXTEK, Inc., Orem, UT
L.V. Knight, S. Cornaby, T. Hughes, A. Stradling, Brigham Young University

F-55 A COMPACT, LOW-POWER TUBE WITH A FIELD EMISSION CATHODE

H.K. Pew, A. Reyes, A. Astle, D.C. Turner, S. Voronov, MOXTEK, Inc., Orem, UT

Plenary Session
Wednesday, 2 August
(Evergreen Ballroom)

X-ray Analysis in the 21st Century

8:30 a.m. – 12 noon

Organized by: **R. Jenkins,** International Centre for Diffraction Data, Newtown Square, PA
P.K. Predecki, University of Denver, Denver, CO

8:30 WELCOMING REMARKS

Ron Jenkins, Chairman, Denver X-ray Conference, International Centre for Diffraction Data, Newtown Square, PA

IXAS UPDATE

R.L. Snyder, The Ohio State University, Columbus, OH

PRESENTATION OF AWARDS

- 2000 Birks Award to **Yohichi Gohshi,** National Institute for Environmental Studies, Tsukuba, Japan

  Presented by: **Horst Ebel,** Technische Universität Wien, Austria

- Announcement of the 2000 Jerome B. Cohen Student Award

  Presented by: **I. Cev Noyan,** IBM, Yorktown Heights, NY

PLENARY SESSION REMARKS

R. Jenkins, International Centre for Diffraction Data, Newtown Square, PA

P.K. Predecki, University of Denver, Denver, CO

THE FOLLOWING ARE INVITED PAPERS:

9:00 P-1 CHALLENGES FOR X-RAY TECHNIQUES IN THE MICROELECTRONICS INDUSTRY

I.C. Noyan, IBM, Yorktown Heights, NY

9:40 P-2 POTENTIAL OF NOVEL X-RAY TECHNIQUES FOR THE SURFACE EXAMINATION OF MATERIALS

D.K. Bowen, Bede Scientific, Inc., Englewood, CO

10:20 Break

10:40 P-3 WHAT DOES THE RECENT LITERATURE ON X-RAY EMISSION ANALYSIS TELL US ABOUT THE FUTURE?

R. van Grieken, University of Antwerp, Antwerp, Belgium

11:20 P-4 APPLICATIONS OF FUNDAMENTAL PARAMETERS IN X-RAY FLUORESCENCE ANALYSIS

B. Vrebos, Philips Analytical, Almelo, The Netherlands

XRD & XRF

Session C-1 PROBLEMS & SOLUTIONS IN XRD/XRF

Organized by: **V.E. Buhrke,** The Buhrke Company, Portola Valley, CA
D.K. Smith, Emeritus, The Pennsylvania State University, University Park, PA

1:30 D-114 COMPUTATIONAL MATERIALS DESIGN – Invited

R.L. Snyder, The Ohio State University, Columbus, OH

2:00 DATA MINING USING THE NEW ICDD RELATIONAL DATABASE FOR THE POWDER DIFFRACTION FILE (PDF) – Invited

J. Faber, International Centre for Diffraction Data, Newtown Square, PA

2:30 D-075 INTERFERENCE OF PARAMETRIC X-RAY AND COHERENT BREMSSTRAHLUNG RADIATION FROM NONRELATIVISTIC ELECTRONS: APPLICATION TO THE PHASE ANALYSIS

I.D. Feranchuk, Belorussian State University, Minsk, Republic of Belarus
A. Ulyanenkov, J. Harada, Rigaku Corporation, Tokyo, Japan

2:50 D-087 MAJOR PROBLEMS IN THE CHARACTERIZATION OF THIN FILMS

R. Ortega, Rigaku/USA, The Woodlands, TX
K. Omote, J. Harada, Rigaku Corporation, Tokyo, Japan

3:10 Break

3:40 F-03 FUSION FOR BETTER ANALYTICAL RESULTS

M. Davidts, I.C.P.H. Chemical International, Philadelphia, PA

4:00 F-42 APPROACHING A UNIVERSAL SAMPLE PREPARATION METHOD FOR XRF ANALYSIS OF POWDER MATERIALS

J. Anzelmo, A. Seyfarth, L. Arias, Bruker AXS, Inc., Madison, WI

4:20 C-1 XRD VERSUS XRF FOR CHEMISTRY BATH CONTROL IN ALUMINUM PRODUCTION

S. Kirik, Institute of Chemistry and Chemical Engineering, Krasnoyarsk, Russia
I. Yakimov, Academy of Non-ferrous Metals and Gold, Krasnoyarsk, Russia

Session, Wednesday p.m. (Evergreen B)

XRD

SESSION D-1 RIETVELD ANALYSIS

Organized by: **R.E. Dinnebier,** University of Bayreuth, Bayreuth, Germany

co-Chair: **E. Antipov,** Moscow State University, Moscow, Russia

1:30 D-072 RECENT DEVELOPMENTS OF FullProf: SUPERSTRUCTURE ANALYSIS, GENERALIZED COORDINATES REFINEMENTS, MICROSTRUCTURE MODELS AND FORM FACTORS – Invited

J. Rodríguez-Carvajal, Laboratoire Léon Brillouin (CEA-CNRS), Gif-sur-Yvette, France

2:00 D-113 SOLVING PROTEIN STRUCTURES FROM POWDER DIFFRACTION DATA – Invited

R.B. Von Dreele, Los Alamos National Laboratory, Los Alamos, NM

2:30 MICROSTRUCTURAL PROPERTIES FROM RIETVELD REFINEMENT OF HIGH RESOLUTION POWDER PATTERNS – Invited

P.W. Stephens, State University of New York at Stony Brook, Stony Brook, NY

3:00 Break

3:20 D-020 THE IMPORTANCE OF THE SPECIMEN DISPLACEMENT CORRECTION IN RIETVELD PATTERN FITTING WITH SYMMETRIC REFLECTION-OPTICS DIFFRACTION DATA

B. O'Connor, D. Li, Curtin University of Technology, Perth, Australia
B. Hunter, Lucas Heights Research Laboratories, Menai, Australia

3:40 D-081 X-RAY AND NEUTRON RIETVELD REFINEMENTS OF COMPOUNDS IN THE Sr-R-Cu-O SYSTEM (R = LANTHANIDES)

W. Wong-Ng, Q. Huang, T. Haugan, I. Levin, National Institute of Standards and Technology, Gaithersburg, MD
J. Kaduk, BP-Amoco Research Center, Naperville, IL
J. Dillingham, J. Suh, University of Maryland, College Park, MD
R.A. Young, Georgia Institute of Technology, Atlanta, GA

4:00 D-078 AB-INITIO STRUCTURE SOLUTION OF $Rh_4Bi_2O_{9.33}$ FROM STEP INTENSITY DATA WITH TOPAS

F. Stowasser, Ruhr-Universität-Bochum, Bochum, Germany
C. Renkenberger, Universität Heidelberg, Heidelberg, Germany
A. Kern, Bruker AXS GmbH, Karlsruhe, Germany

4:20 D-006 TEXTURE CHARACTERIZATION IN X-RAY AND NEUTRON POWDER DIFFRACTION DATA USING THE GENERALIZED SPHERICAL-HARMONIC

H. Sitepu, National Institute of Standards and Technology, Gaithersburg, MD and SUNY, Stony Brook, NY
H.J. Prask, M.D. Vaudin, National Institute of Standards and Technology, Gaithersburg, MD

4:40 D-026 MICRO RIETVELD ANALYSIS AND 2D DETECTORS

R.G. Tissot, Sandia National Laboratories, Albuquerque, NM
D.E. Simon, DES Consulting, Broken Arrow, OK

5:00 D-059 TOPAS: A NEW DIMENSION IN XRPD STRUCTURE ANALYSIS

A. Kern, A. Coelho, Bruker AXS GmbH, Karlsruhe, Germany

Session, Wednesday p.m. **(Evergreen C)**

XRD

Session D-2 MESOSTRUCTURE ANALYSIS

Organized by: **R.L. Snyder,** The Ohio State University, Columbus, OH
R. Barton, Jr., DuPont Experimental Station, Wilmington, DE

1:40 D-030 X-RAY DIFFRACTION IMAGING AS A TOOL OF MESOSTRUCTURE ANALYSIS – Invited

J. Fiala, Skoda Research, Ltd., Plzeń, Czech Republic

2:10 D-125 LINE PROFILE ANALYSIS OF POLYMERIC FIBERS – Invited

R. Barton, Jr., DuPont Company–Central Research & Development, Wilmington, DE

2:40 D-057 APPLYING THE RIETVELD METHOD TO A MINERAL FILLED PPS COMPOUND

R.W. Morton, J.F. Geibel, J.J. Gislason, R.L. Heald, Phillips Petroleum Company, Bartlesville, OK
D.E. Simon, DES Consulting, Broken Arrow, OK

3:00 Break

3:30 D-094 WHAT CAN WE LEARN FROM STRAIN ANISOTROPY? – Invited

T. Ungár, Eötvös University Budapest, Hungary

4:00 D-110 ANALYSIS OF SIZE-BROADENED PROFILES USING THE MAXIMUM ENTROPY METHOD

N. Armstrong, J.P. Cline, National Institute of Standards and Technology, Gaithersburg, MD
W. Kalceff, University of Technology, Sydney, Australia

4:20 D-107 AN X-RAY DIFFRACTION STUDY OF TRIPHENYL BASED DISCOTIC LIQUID CRYSTALS

T. Blanton, Eastman Kodak Company, Rochester, NY
S.H. Chen, J. Mastrangelo, P. Chen, University of Rochester, Rochester, NY

4:40 D-040 X-RAY MICROBEAM DIFFRACTION COMPARISON OF MESOTEXTURES IN PLATES OF THREE ALUMINUM ALLOYS

K. Ignatiev, S.R. Stock, Georgia Institute of Technology, Atlanta, GA
Z.U. Rek, Stanford Synchrotron Radiation Laboratory, Stanford, CA

5:00 D-079 ANALYSIS OF STRAIN ANISOTROPHY IN DELTA STABILIZED Pu-Ga ALLOYS

L. Morales, A. Lawson, J. Kennison, Los Alamos National Laboratory, Los Alamos, NM

XRF

SESSION F-1 INDUSTRIAL APPLICATIONS OF XRF I

Organized by: **R. Wilson,** Rigaku/USA, Inc., Danvers, MA
D. Broton, Construction Technology Laboratories, Skokie, IL

1:30 F-34 SILICON TO TUNGSTEN RATIO DETERMINATION IN TUNGSTEN SILICIDE USING XRF – Invited

M. Godbole, Dominion Semiconductor LLC, Manassas, VA

2:00 F-10 ACCURATE QUANTIFICATION OF DRIED RESIDUE THIN FILMS USING X-RAY FLUORESCENCE

C.G. Worley, G.J. Havrilla, Los Alamos National Laboratory, Los Alamos, NM

2:20 F-14 THICKNESS AND COMPOSITION ANALYSIS OF BST FILM USING XRF — THE USE OF A GONIOMETER WITH A BACKGROUND MEASUREMENT MECHANISM

S. Fujimura, H. Homma, H. Kobayashi, H. Kohno, Rigaku Industrial Corporation, Japan
R. Wilson, Rigaku/USA, Inc., Danvers, MA

2:40 F-48 COMPARISON OF THREE UNIVERSAL CURVES FOR THE ESCAPE PROBABILITY OF X-RAY EXCITED ELECTRONS: I. THEORY

H. Ebel, R. Svagera, M.F. Ebel, W.S.M. Werner, Technische Universität Wien, Wien, Austria

3:00 Break

3:20 F-49 COMPARISON OF THREE UNIVERSAL CURVES FOR THE ESCAPE PROBABILITY OF X-RAY EXCITED ELECTRONS: II. EVALUATION OF LAYER THICKNESSES DETERMINED BY TOTAL ELECTRON YIELD (TEY)

H. Ebel, R. Svagera, M.F. Ebel, W.S.M. Werner, Technische Universität Wien, Wien, Austria

3:40 THE CHALLENGES OF SAMPLING AND SPECIMEN PREPARATION OF ALTERNATE RAW MATERIALS IN THE CEMENT INDUSTRY – Invited

D. Broton, Construction Technology Laboratories, Skokie, IL

4:10 F-20 DEVELOPMENT OF SRM® 2780 HARD ROCK MINE WASTE – Invited

J. Sieber, G. Turk, M. Epstein, C. Beck II, A. Marlow, National Institute of Standards and Technology, Gaithersburg, MD
S. Wilson, J. Taggart, United States Geological Survey

4:40 F-02 THE PRESENT STATUS AND FEATURES OF GEOCHEMICAL MAPPING USING X-RAY FLUORESCENCE SPECTROMETRY IN CHINA

G. Ma, G. Ling, L. Luo, National Research Center of Geological Analysis, Beijing, China
G. Li, Institute of Geophysical and Geochemical Exploration, Hebei, China

5:00 F-40 PORTABLE XRF INSTRUMENTATION FOR MINING

D.J. Watson, T. Howe, D. Kenning, Edax Portable Products Division, Kennewick, WA
J. Nicolosi, Edax, Inc., Mahwah, NJ

XRD & XRF

Session C-2 MICROBEAM TECHNIQUES I

Organized by: **G.E. Ice,** Oak Ridge National Laboratory, Oak Ridge, TN
I.C. Noyan, IBM, Yorktown Heights, NY

8:40 D-108 WHITE AND MONOCHROMATIC X-RAY MICROBEAM INVESTIGATIONS OF MATERIALS MICROSTRUCTURE AND TRI-AXIAL STRESS/STRAIN ON MESOSCOPIC LENGTH SCALES – Invited

B.C. Larson, Oak Ridge National Laboratory, Oak Ridge, TN

9:10 HARD X-RAY MICROSCOPY: COMBINATION OF MICRODIFFRACTION, MICROSPECTROSCOPY AND PHASE CONTRAST IMAGING – Invited

A. Snigirev, European Synchrotron Radiation Facility, Grenoble, France

9:40 F-09 CAPILLARY MICRO X-RAY FLUORESCENCE OF PARTICLES USING LABORATORY X-RAY TUBES

J.R. Swider, T. Jach, E. Steel, National Institute of Standards and Technology, Gaithersburg, MD

10:00 Break

10:30 F-28 APPLICATIONS OF IN SITU MICRO-EDXRF IN PHILATELY

G.S. Hall, Rutgers University, Piscataway, NJ
B. Scruggs, EDAX International

10:50 F-30 SMALL SPOT X-RAY ANALYSIS WITH CCD MAPPING CAPABILITIES

H. Inoue, Y. Yamada, M. Inoue, K. Okuda, Rigaku Industrial Corp., Osaka, Japan
G. Hamill, J. Martin, Rigaku/USA, Inc., Danvers, MA

11:10 F-37 ELEMENTAL SCREENING OF COMBINATORIAL CHEMICAL LIBRARIES USING MICRO X-RAY FLUORESCENCE

G.J. Havrilla, G. Mann, B. Warner, Los Alamos National Laboratory, Los Alamos, NM

11:30 C-2 RECENT DEVELOPMENTS IN X-RAY OPTICS FOR XRD & XRF INSTRUMENTATION

M. Haller, Z. Chen, N. Gao, M. McColgan, J. Nicolich, X-ray Optical Systems, Inc., Albany, NY

XRD

Session D-3 JEROME B. COHEN COMMEMORATIVE SESSION I: STRESS ANALYSIS BY DIFFRACTION METHODS I AND TEXTURE

Organized by: **J. Fiala,** SKODA Research, Ltd., Plzeń, Czech Republic

co-Chair: **R.A. Winholtz,** University of Missouri, Columbia, MO

8:30 Introduction by **Aaron Krawitz,** University of Missouri, Columbia, MO, former student of Jerome Cohen

9:00 D-012 X-RAY STRESS ANALYSIS IN PRESENCE OF GRADIENTS AND TEXTURE – Invited

Ch. Genzel, Hahn-Meitner-Institut, Berlin, Germany

9:30 D-017 PROGRESS IN THE X-RAY DIFFRACTION OF THE RESIDUAL MACRO-STRESSES DETERMINATION RELATED TO SURFACE LAYER GRADIENTS AND ANISOTROPY – Invited

S.J. Skrzypek, A. Baczmański, University of Mining and Metallurgy-AGH, Kraków, Poland

10:00 Break

10:20 D-119 CALCULATION OF MAJOR CRYSTALLOGRAPHIC POLES ALONG ODF FIBERS PARALLEL TO THE GAMMA FIBER – Invited

S.H. Magner, B.M. Wilson, University of Nebraska, Lincoln, NE
R.J. De Angelis, University of Florida, Shalimar, FL

10:50 D-090 STRESS ANALYSIS OF THIN FILMS OF IRON AND COBALT STEEL ALLOYS USING A 4x10 mm^2 MONOCHROMATIC Cr Kα BEAM FROM A 100 mm LONG PARABOLIC MULTILAYER OPTIC

H. Zadoori, B.R. York, Q.-F. Xiao, IBM Materials Laboratory, San Jose, CA
Z. Al-Mosheky, L. Jiang, Osmic, Inc., Troy, MI

11:10 D-051 STRESS AND TEXTURE ANALYSIS WITH TWO-DIMENSIONAL DETECTORS

B.B. He, U. Preckwinkel, K. Smith, Bruker Analytical X-ray Systems, Madison, WI

11:30 D-037 THERMAL EXPANSION MEASUREMENTS OF LATTICE PARAMETERS USING PARALLEL-BEAM POWDER DIFFRACTOMETRY

T. Mitsunaga, M. Saigo, G. Fujinawa, J. Harada, Rigaku Corporation, Tokyo, Japan

11:50 D-019 INFLUENCE OF TEXTURE AND ANISOTROPHY ON MICROSTRESSES AND FLOW BEHAVIOR IN A DUPLEX STAINLESS STEEL DURING LOADING

J. Johansson Moverare, M. Odén, Linkoping University, Linköping, Sweden

12:10 D-106 RESIDUAL STRESSES IN TUNGSTEN/BULK METALLIC GLASS COMPOSITES

D. Dragoi, E. Üstündag, California Institute of Technology, Pasadena, CA
B. Clausen, M.A.M. Bourke, Los Alamos National Laboratory, Los Alamos, NM
J.W. Richardson, Jr., Argonne National Laboratory, Argonne, IL

XRD

Session D-4 PHASE TRANSFORMATIONS AND REACTIONS I

Organized by: **E. Üstündag,** California Institute of Technology, Pasadena, CA

co-Chair: **M.A.M. Bourke,** Los Alamos National Laboratory, Los Alamos, NM

8:30 D-109 HIGH TEMPERATURE, DISPLACIVE TRANSFORMATIONS IN OXIDE CERAMICS – Invited

W.M. Kriven, University of Illinois at Urbana-Champaign, Urbana, IL

9:00 D-115 PHASE RELATIONSHIPS IN Sr-Fe-Co-O PEROVSKITE-BASED CERAMIC MEMBRANES – Invited

J.W. Richardson, Jr., B.J. Mitchell, C.D. Murphy, G. Ma, Argonne National Laboratory, Argonne, IL

9:30 D-104 INVESTIGATION OF THE REDUCTION OF $NiAl_2O_4$

D. Dragoi, E. Üstündag, J.C. Hanan, California Institute of Technology, Pasadena, CA
B. Clausen, M.A.M. Bourke, Los Alamos National Laboratory, Los Alamos, NM
J.W. Richardson, Jr., Argonne National Laboratory, Argonne, IL

9:50 D-105 EFFECT OF PRESSURE ON THE STRUCTURE OF $NiAl_2O_4$

I. Halevy, E. Üstündag, J.C. Hanan, D. Dragoi, California Institute of Technology, Pasadena, CA
J. Hu, NSLS, Brookhaven National Laboratory, Upton, NY

10:10 Break

10:40 D-031 STUDY AND SIMULATION OF ORDER-DISORDER TRANSITIONS IN BROWNMILLERITE-TYPE CONDUCTING CERAMICS

S.A. Speakman, S.T. Misture, New York State College of Ceramics at Alfred University, Alfred, NY

11:00 D-027 FERROELECTRIC PHASE TRANSITIONS IN Nb-doped $KTiOPO_4$

S.A. Ivanov, S.Yu. Stefanovich, Karpov' Institute of Physical Chemistry, Moscow, Russia
S.-G. Eriksson, University of Gothenburg, Studsvik, Sweden
V.I. Voronkova, T.Yu. Losevskaya, V.K. Yanovskii, Moscow State University, Moscow, Russia
R. Tellgren, H. Rundlöf, Uppsala University, Uppsala, Sweden

11:20 D-102 CORRELATIONS BETWEEN BOEHMITE CRYSTAL SIZE AND ALUMINA PROPERTIES

X. Bokhimi, M.L. Guzmán-Castillo, F. Hernández-Beltrán, J. Salmones-Blásquez, A. Toledo, Instituto Mexicano del Petróleo, Mexico

11:40 D-055 INVESTIGATION OF GLASS BATCH REACTIONS AT RAPID HEATING RATES USING AN IN SITU DIFFRACTION FURNACE

M. Kolb, S.T. Misture, New York State College of Ceramics at Alfred University, Alfred, NY

XRF

Session F-2 NEW DEVELOPMENTS IN XRF I

Organized by: **V.E. Buhrke,** The Buhrke Company, Portola Valley, CA
M.A. Zaitz, IBM Microelectronics, Hopewell Junction, NY

9:00 F-27 LIMITS OF SENSITIVITY FOR SYNCHROTRON RADIATION TXRF – Invited

P. Pianetta, K. Baur, S. Brennan, A. Singh, Stanford Synchrotron Radiation Laboratory, Stanford, CA

9:30 F-43 TXRF – TRENDS AND DEVELOPMENTS – Invited

A. Aiginger, C. Streli, P. Wobrauschek, Atominstitut der Österreichischen Universitäten, Vienna, Austria

10:00 Break

10:30 F-51 SYNCHROTRON RADIATION INDUCED TXRF OF “LAM” STEEL SAMPLES

P. Wobrauschek, G. Pepponi, C. Streli, N. Zöger, Atominstitut der Österreichischen Universitäten, Vienna, Austria
F. Hegedüs, C. Hegedüs, X-ray Consulting c/o EPFL-CRPP, Villigen PSI, Switzerland

10:50 F-45 SYNCHROTRON RADIATION INDUCED TXRF OF LOW Z ELEMENTS AT SSRL AND AT THE PTB BEAMLINE AT BESSY2

C. Streli, P. Wobrauschek, P. Kregsamer, G. Pepponi, Atominstitut der Österreichischen Universitäten, Vienna, Austria
B. Beckhoff, G. Ulm, Physikalisch-Technische Bundesanstalt, Berlin, Germany
P. Pianetta, Stanford Synchrotron Radiation Laboratory, Stanford, CA
S. Pahlke, L. Fabry, Wacker Siltronic AG, Burghausen, Germany

11:10 F-13 CONTAMINATION ANALYSIS OF Cu INTERCONNECT PROCESS SAMPLES BY TXRF

H. Kohno, M. Matsuo, H. Kohno, Rigaku Industrial Corporation
R. Wilson, Rigaku/USA, Inc., Danvers, MA

11:30 F-04 TRACE ELEMENTS IN LIGHT MATRICES USING XRF: COMPARISON OF DIFFERENT ANALYTICAL METHODS AND INSTRUMENTS

D. Bonvin, A. Kohler, R. Yellepeddi, ARL Applied Research Laboratories SA, Ecublens, Switzerland

XRD & XRF

SESSION C-3 MICROBEAM TECHNIQUES II

Organized by: **G.E. Ice,** Oak Ridge National Laboratory, Oak Ridge, TN
I.C. Noyan, IBM, Yorktown Heights, NY

2:00 D-073 THREE VIEWS OF THE MOSAIC STRUCTURE IN RELAXED SiGe/Si HETEROSTRUCTURES

J.L. Jordan-Sweet, P.M. Mooney, I.C. Noyan, S.K. Kaldor, IBM Research Division, Yorktown Heights, NY
P.-C. Wang, IBM Microelectronics Division, Hopewell Junction, NY
B. Lai, Z. Cai, P. Illinski, D. Legnini, W. Rodrigues, Argonne National Laboratory, Argonne, IL
C. Stagarescu, X. Su, G. Xu, D.E. Eastman, University of Chicago, Chicago, IL

2:20 D-058 COMPARISON OF LABORATORY-BASED X-RAY MICRODIFFRACTION AND ELECTRON BACKSCATTER DIFFRACTION FOR PHASE IDENTIFICATION

J.R. Verkouteren, J.A. Small, National Institute of Standards and Technology, Gaithersburg, MD

2:40 D-028 MICRO-DIFFRACTION WITH MONO-CAPILLARIES

M.J. Fransen, J.H.A. Vasterink, J. te Nijenhuis, Philips Analytical, Almelo, The Netherlands

3:00 Break

3:30 D-025 IN SITU STUDIES OF POLYCRYSTALLINE DEFORMATION USING HIGH ENERGY FOCUSED X-RAYS

L. Margulies, RISØ National Laboratory, Roskilde, Denmark and ESRF, Grenoble, France
H.F. Poulsen, D.J. Jensen, T. Lorentzen, RISØ National Laboratory, Roskilde, Denmark
U. Lienert, A. Kvick, ESRF, Grenoble, France

3:50 D-100 TEXTURE MEASUREMENTS IN Cu DAMASCENE INTERCONNECT LINES FOR NEW LOGIC TECHNOLOGIES USING AN IMAGE PLATE

D. Winter, Rigaku/USA, Inc., The Woodlands, TX
Q.-T. Jiang, International Sematech, Austin, TX
P. Besser, Motorola-AMD Alliance Technology

4:10 D-099 MECHANICAL STRESS IN Al AND Cu DAMASCENE INTERCONNECT LINES USING IN SITU HIGH TEMPERATURE MICRO-BEAM TECHNIQUES

D. Winter, Rigaku/USA, Inc., The Woodlands, TX
P. Besser, Motorola-AMD Alliance Technology
Q.-T. Jiang, International Sematech, Austin, TX

4:30 D-117 RESIDUAL STRESSES IN Ti-SiC COMPOSITES

J.C. Hanan, D. Dragoi, E. Üstündag, California Institute of Technology, Pasadena, CA
I.C. Noyan, IBM, Yorktown Heights, NY

XRD

Session D-5 JEROME B. COHEN COMMEMORATIVE SESSION II: STRESS ANALYSIS BY DIFFRACTION METHODS II

Organized by: **P.K. Predecki,** University of Denver, Denver, CO

2:00 D-116 ENGINEERING APPLICATIONS OF X-RAY STRESS ANALYSIS – Invited

N. Ganev, I. Kraus, Czech Technical University, Prague, Czech Republic

2:30 D-112 MODELING FATIGUE CRACK PROPAGATION IN THE PRESENCE OF RESIDUAL STRESS – Invited

R.A. Winholtz, University of Missouri, Columbia, MO

3:00 D-084 VAMAS STANDARDS DEVELOPMENT FOR NEUTRON DIFFRACTION STRAIN MAPPING

X.-L. Wang, D. Wang, S. Spooner, C.R. Hubbard, Oak Ridge National Laboratory, Oak Ridge, TN

3:20 Break

3:50 D-005 NUMERICAL SIMULATION OF THE X-RAY STRESS ANALYSIS TECHNIQUE IN POLYCRYSTALLINE MATERIALS WITH HEXAGONAL CRYSTAL SYMMETRY

H. Wern, T. Maas, N. Koch, HTW des Saarlandes, Saarbrücken, Germany

4:10 D-016 AN ELASTIC CONSTANTS DATABASE AND XEC CALCULATOR FOR USE IN XRD RESIDUAL STRESS ANALYSIS

A.C. Vermeulen, Philips Analytical, Almelo, The Netherlands

4:30 D-035 EVALUATION OF RESIDUAL STRESSES IN COMPOSITE TUBING UNDER THERMAL LOADING WITH MECHANICAL CONSTRAINT USING NEUTRON DIFFRACTION AND FINITE ELEMENT METHODS

T. Ely, X.-L. Wang, G. Sarma, C. Hubbard, Oak Ridge National Laboratory, Oak Ridge, TN

4:50 D-052 RESIDUAL STRAINS IN WELDED Be RINGS

D.W. Brown, R. Varma, M.A.M. Bourke, P. Burgardt, F. Guerra, Los Alamos National Laboratory, Los Alamos, NM

5:10 D-043 STUDY AND SERVICE CONTROL OF STRESS STATE OF HIGH-STRENGTH STEEL CABLES, USED IN PRESTRESSED CONCRETE STRUCTURES

V. Monine, Instituto Politécnico do Rio de Janeiro, Nova Friburgo, Brasil
T. Gurova, J.R. Teodósio, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brasil

XRD

Session D-6 PHASE TRANSFORMATIONS AND REACTIONS II

Organized by: **E. Üstündag,** California Institute of Technology, Pasadena, CA

co-Chair: **M.A.M. Bourke,** Los Alamos National Laboratory, Los Alamos, NM

2:00 D-045 STRAIN, TEXTURE AND PHASE-FRACTION MEASUREMENTS DURING STRESS-INDUCED TRANSFORMATIONS IN SHAPE-MEMORY MATERIALS – Invited

R. Vaidyanathan, Massachusetts Institute of Technology, Cambrige, MA
D.C. Dunand, Department of Materials Science & Engineering, Northwestern University
M.A.M. Bourke, Los Alamos National Laboratory, Los Alamos, NM

2:30 D-046 NON-DESTRUCTIVE IN SITU REAL-TIME MEASUREMENTS OF STRUCTURAL PHASE TRANSITIONS USING NEUTRON TRANSMISSION – Invited

S. Vogel, H.-G. Priesmeyer, Christian-Albrechts-Universität Kiel, Kiel, Germany
M. Bourke, Los Alamos National Laboratory, Los Alamos, NM
E. Üstündag, California Institute of Technology, Pasadena, CA

3:00 Break

3:20 D-103 INVESTIGATION OF REACTION KINETICS USING NEUTRON SCATTERING

E. Üstündag, J.C. Hanan, D. Dragoi, California Institute of Technology, Pasadena, CA
B. Clausen, M.A.M. Bourke, Los Alamos National Laboratory, Los Alamos, NM
J.W. Richardson, Jr., Argonne National Laboratory, Argonne, IL
S. Vogel, Christian-Albrechts-Universität Kiel, Germany

3:40 D-047 AUTOMATED RIETVELD-ANALYSIS OF LARGE NUMBERS OF DATASETS

S. Vogel, H.-G. Priesmeyer, Christian-Albrechts-Universität Kiel, Kiel, Germany

4:00 D-054 SYNCHROTRON X-RAY POWDER DIFFRACTION STUDIES OF MORDENITE CATALYSTS

C.E. Crowder, A. Kuperman, The Dow Chemical Company, Midland, MI

4:20 D-007 BULK MODULUS AND HIGH PRESSURE CRYSTAL STRUCTURES OF $C(Si(CH_3)_3)_4$ DETERMINED BY X-RAY POWDER DIFFRACTION

R.E. Dinnebier, S. van Smaalen, University of Bayreuth, Bayreuth, Germany
S. Carlson, ESRF, Grenoble, France

4:40 D-013 REAL-TIME SYNCHROTRON X-RAY POWDER DIFFRACTION STUDY OF THE STRUCTURE AND DEHYDRATION OF TODOROKITE

J.E. Post, Smithsonian Institution, Washington, DC
P.J. Heaney, The Pennsylvania State University, University Park, PA
and Brookhaven National Laboratory, Upton, NY

5:00 D-074 THE ELECTRON DENSITY DISTRIBUTION OF TETRAGONAL $BaTiO_3$ OBTAINED BY THE MAXIMUM ENTROPY METHOD

J. Harada, K. Yugami, Rigaku Corporation, Tokyo, Japan
M. Sakata, E. Nishibori, M. Takata, Nagoya University, Nagoya, Japan
Y. Akishige, T. Nakata, Shimane University, Matsue, Japan
Y. Kuroiwa, Okayama University, Okayama, Japan

XRD

Session D-7 NEW DEVELOPMENTS IN XRD INSTRUMENTATION I

Organized by: **S.T. Misture,** New York State College of Ceramics at Alfred University, Alfred, NY

co-Chair: **T. Ungár,** Eötvös University Budapest, Hungary

1:30 D-111 HIGH ACCURACY LATTICE PARAMETER MEASUREMENTS – Invited

J.P. Cline, R.D. Deslattes, J.-L. Staudenmann, E.G. Kessler, L.T. Hudson, A. Henins, National Institute of Standards and Technology, Gaithersburg, MD
R.W. Cheary, University of Technology, Sydney, Australia

2:00 D-029 WHAT CAN YOUR DIFFRACTOMETER DO FOR YOU? CROSS TECHNIQUE MATERIAL ANALYSIS WITH ONE MACHINE

C.H. Russell, S.M. Owens, R.D. Deslattes, National Institute of Standards and Technology, Gaithersburg, MD

2:20 D-089 LATEST DEVELOPMENT OF MULTILAYER COLLIMATING AND FOCUSING OPTICS

B. Verman, L. Jiang, B. Kim, S. Seshadri, D. Wilcox, N. Grupido, Osmic, Inc., Troy, MI

2:40 D-077 TOROIDAL FOCUSING OPTIC FOR µXRD STRESS MEASUREMENTS

Q.-F. Xiao, B. York, H. Zadoori, IBM Materials Laboratory, San Jose, CA
Z. Chen, X-ray Optical Systems, Albany, NY

3:00 Break

3:30 D-014 CHARACTERIZATION OF X-RAY DIFFRACTION SYSTEM WITH A MICRO-FOCUS X-RAY SOURCE AND A POLYCAPILLARY OPTIC

M. Gubarev, M. Joy, NASA/Marshall Space Flight Center, Huntsville, AL
E. Ciszak, NASA/Marshall Space Flight Center, Huntsville, AL and Universities Space Research Association, Huntsville, AL
I. Ponomarev, X-ray Optical Systems, Inc., Albany, NY

3:50 D-093 A PARALLEL BEAM GEOMETRY FOR ACCURATE PHASE ANALYSIS

J. te Nijenhuis, V.A. Kogan, Philips Analytical, Almelo, The Netherlands

4:10 D-086 IMAGING PLATE SYSTEMS FOR DIFFRACTION D/MAX-Rapid, R/AXIS-Rapid

R. Ortega, Rigaku/USA, The Woodlands, TX
K. Masuda, J. Harada, Rigaku Corporation, Tokyo, Japan

4:30 D-044 NEW REFLECTION METHOD FOR THE DETERMINATION OF A COMPLETE POLE FIGURE

R. Yokoyama, K. Oguiso, Rigaku Corporation, Tokyo, Japan

4:50 D-053 XRD RAPID SCREENING SYSTEM FOR COMBINATORIAL CHEMISTRY

B.B. He, J. Anzelmo, P. LaPuma, U. Preckwinkel, K. Smith, Bruker Analytical X-ray Systems, Madison, WI

XRF

Session F-3 NEW DEVELOPMENTS IN XRF II

Organized by: **V.E. Buhrke,** The Buhrke Company, Portola Valley, CA
M.A. Zaitz, IBM Microelectronics, Hopewell Junction, NY

2:00 F-08 BRAGG POLARIZATION OPTICS IN EDXRF

J. Heckel, SPECTRO A.I., Kleve, Germany

2:20 F-22 EXAMINATION OF POLYCAPILLARY LENSES FOR MICRO-XRF

M. Haschke, P. Pfannekuch, Röntgenanalytik Messtechnik GmbH, Germany
B. Scruggs, EDAX, Inc.

2:40 F-38 MICRO X-RAY FLUORESCENCE WITH MONOLITHIC POLYCAPILLARY OPTICS

G.J. Havrilla, Los Alamos National Laboratory, Los Alamos, NM

3:00 Break

3:30 F-47 DOUBLY CURVED CRYSTAL OPTICS AND THEIR APPLICATIONS

Z.W. Chen, J.P. Nicolich, X-ray Optical Systems, Inc., Albany, NY

3:50 C-4 INNOVATIVE PRODUCTS FOR XRF AND XRD SAMPLE PREPARATION

M. Dessureault, Corporation Scientifique Claisse, Inc., Quebec, Canada
R. Bostwick, SPEX CertiPrep, Inc., Metuchen, NJ

4:10 F-52 THE NEW COMPACT “PLUG AND PLAY” WDXRF CONCEPT

J.A. Anzelmo, Bruker AXS, Inc., Madison, WI

4:30 F-23 A COMPACT X-RAY SPECTROMETER WITH MULTI-CAPILLARY X-RAY LENS AND FLAT CRYSTALS

H. Soejima, Shimadzu Scientific Research, Kyoto, Japan
T. Narusawa, Kochi University of Technology, Kochi, Japan

XRD

Session D-8 NEW DEVELOPMENTS IN XRD INSTRUMENTATION II

Organized by: **S.T. Misture,** New York State College of Ceramics at Alfred University, Alfred, NY

co-Chair: **B. O'Connor,** Curtin University of Technology, Perth, Australia

8:30 D-004 RAY-TRACING STUDY ON A $K\alpha_1$-$K\alpha_2$ CHARACTERISTIC OF A PARABOLIC GRADED MULTILAYER – Invited

H. Toraya, Nagoya Institute of Technology, Tajimi, Japan

9:00 D-018 WAVELET REPRESENTATION OF DIFFRACTION POLE FIGURES

H. Schaeben, J. Prestin, Freiberg University of Mining and Technology, Freiberg, Germany

9:20 D-095 AN INSTRUMENT FOR RAPID TEXTURE MAPPING ON 200 MM WAFERS

K.J. Kozaczek, R.I. Martin, D.S. Kurtz, P.R. Moran, S.P. O'Leary, HyperNex, Inc., State College, PA

9:40 D-118 INNOVATIVE ADVANCES IN THE FIELD OF X-RAY DIFFRACTION ANALYSIS

P.J. LaPuma, Bruker AXS, Inc., Billerica, MA

10:00 Break

10:20 D-041 PORTABLE MINIDIFFRACTOMETER FOR MEASUREMENTS IN-LABORATORY AND IN-FIELD CONDITIONS

J.T. de Assis, V.I. Monine, F.R. Pereira, Instituto Politécnico do Rio de Janeiro, Nova Friburgo, Brasil

10:40 D-101 MNI, A NEW APPROACH TO QUANTITATIVE XRD ANALYSIS USING THE ICDD PDF-2 DATABASE

R. Clapp, Diffraction Technology Pty. Ltd., Canberra, Australia

11:00 D-092 NEW DEVELOPMENTS IN (OLD) XRD SOFTWARE: JPOWD

Q. Johnson, S. Weber, Materials Data, Inc., Livermore, CA

11:20 D-061 TRADITIONAL ANALYTICAL X-RAY TECHNIQUE INITIATES INNOVATIVE DEVELOPMENTS OF INDUSTRIAL SYSTEMS IN AIRCRAFT, SEMICONDUCTOR AND AUTOMOTIVE QUALITY CONTROL

A. Haase, Rich. Seifert & Co., Ahrensburg, Germany

XRD

Session D-9 THIN FILMS ANALYSIS XRD

Organized by: **T.C. Huang,** Emeritus, IBM Almaden Research Center, San Jose, CA

co-Chairs: **J. Harada,** Rigaku Corporation, Tokyo, Japan
S.-F. Lin, Nankai University, Tianjin, People's Republic of China

8:30 D-080 X-RAY CHARACTERIZATION OF SURFACE AND INTERFACE ROUGHNESS – Invited

J. Harada, Rigaku Corporation, Tokyo, Japan

9:00 D-091 NEW ANALYTICAL PROCEDURE FOR DETERMINING THE CRYSTALLITE SIZE DISTRIBUTION THROUGH PROFILE FITTING

B.R. York, IBM Materials Laboratory, San Jose, CA

9:20 D-039 X-RAY STUDY OF Mo/Si MULTILAYERS GROWN ON GLASS SUBSTRATE

A. Ulyanenkov, K. Inaba, K. Omote, J. Harada, Rigaku Corporation, Tokyo, Japan
M. Ishino, O. Yoda, Advanced Photon Research Center, Kyoto, Japan

9:40 D-011 IN SITU X-RAY DIFFRACTION ANALYSIS OF DISORDER AND STRAIN IN ION IMPLANTED CERAMIC THIN FILMS

S. Grigull, European Synchrotron Radiation Facility, Grenoble, France
M. Nastasi, Los Alamos National Laboratory, Los Alamos, NM
C.A. Zorman, Case Western Reserve University, Cleveland, OH

10:00 Break

10:20 D-038 X-RAY DIFFRACTION ANALYSIS OF FREE-STANDING AND BURIED QUANTUM WIRES – Invited

A. Ulyanenkov, K. Omote, K. Inaba, Rigaku Corporation, Tokyo, Japan
U. Pietsch, N. Darowski, University of Potsdam, Potsdam, Germany
P. Mikulik, Masaryk University, Brno, Czech Republic
A. Forchel, University of Wurzburg, Wurzburg, Germany

10:50 D-097 HIGH RESOLUTION TEXTURE ANALYSIS OF THIN BLANKET FILMS DISCREET TEST STRUCTURES IN SEMICONDUCTOR DEVICES

K.J. Kozaczek, R.I. Martin, D.S. Kurtz, P.R. Moran, S.P. O'Leary, HyperNex, Inc., State College, PA

11:10 D-050 AN INVESTIGATION OF GIANT MAGNETORESISTANCE (GMR) SPIN-VALVE STRUCTURES USING X-RAY DIFFRACTION AND REFLECTIVITY

E. Brown, EB Scientific Enterprises, Golden, CO
M. Wormington, Bede Scientific Incorporated, Englewood, CO

11:30 D-088 APPLICATIONS OF FAST X-RAY REFLECTOMETRY – A NEW TOOL FOR IN SITU THIN FILM ANALYSIS

D.K. Agnihotri, R. Ortega, Rigaku/USA, The Woodlands, TX

XRF

Session F-4 INDUSTRIAL APPLICATIONS OF XRF II

Organized by: **H.L. Baker,** Northwest Alloys (ALCOA), Addy, WA
G.J. Havrilla, Los Alamos National Laboratory, Los Alamos, NM

8:00 F-06 PROBLEMS BY USING PRESSED POWDER PELLETS FOR XRF ANALYSIS OF FERROSILICON ALLOYS – Invited

T. Eivindson, Ø. Mikkelsen, Elkem ASA Research, Norway

8:30 ANALYSIS OF NICKEL, CHROME AND FERROUS BASED METALS BY XRF USING FUNDAMENTAL PARAMETERS APPROACH – Invited

B. Wheeler, Rigaku/USA, Inc. (retired), Danvers, MA

9:00 F-11 FUSED BEADS FROM METAL DRILLINGS AND CHIPS APPLICATION TO Sn-Pb ALLOYS

J. Blanchette, F. Claisse, Corporation Scientifique Claisse, Inc., Québec, Canada

9:20 F-29 APPLICATIONS OF X-RAY ANALYSES AS A PROCESS MONITORING TOOL IN ALUMINIUM INDUSTRY

K.V. Krishnan, V.V. Kutumbarao, Jawaharlal Nehru Aluminium Research Development and Design Centre, Nagpur, India

9:40 F-35 XRF'S ROLE IN THE PRODUCTION OF MAGNESIUM METAL BY THE MAGNATHERMIC METHOD

H.L. Baker, Northwest Alloys, Inc., Addy, WA

10:00 Break

10:20 F-39 PORTABLE XRF FOR METALS ANALYSIS

D. Kenning, R. Kuhlman, L.S. Price, Edax Portable Products Division, Kennewick, WA
J. Nicolosi, R. Shen, Edax, Inc., Mahwah, NJ

10:40 F-41 REFINEMENTS USEFUL FOR X-RAY FLUORESCENCE CALIBRATION CURVES – Invited

R.W. Morton, J.F. Geibel, J.J. Gislason, R.L. Heald, Phillips Petroleum Company, Bartlesville, OK

11:10 F-19 CERTIFICATION OF SRM® 1848 PCMO ADDITIVE PACKAGE

J. Sieber, S. Leigh, National Institute of Standards and Technology, Gaithersburg, MD

XRF

SESSION F-5 QUANTITATIVE XRF & SOFTWARE

Organized by: **M. Mantler,** Vienna University of Technology, Vienna, Austria

co-Chair: **R. van Grieken,** University of Antwerp, Antwerp, Belgium

8:30 F-44 QUANTITATIVE XRF OF ART OBJECTS – Invited

M. Schreiner, Academy of Fine Arts, Vienna, Austria
C. Neelmeijer, Research Center Rossendorf, Inc., Dresden, Germany
M. Mantler, Vienna University of Technology, Vienna, Austria

9:00 F-24 INVESTIGATION OF FLUORESCENCE YIELDS OF LOW Z ELEMENTS USING MONOCHROMATIZED SYNCHROTRON RADIATION OF HIGH SPECTRAL PURITY – Invited

B. Beckhoff, G. Ulm, Physikalisch-Technische Bundesanstalt, Berlin, Germany

9:30 F-05 A CRITICAL EVALUATION OF LINE OVERLAP CORRECTIONS IN X-RAY SPECTROMETRY

L.E. Creasy, Titanium Metals Corporation, Morgantown, PA

9:50 F-15 NEW APPLICATIONS OF MULTIFUNCTIONAL SYSTEM OF ENERGY DISPERSIVE X-RAY FLUORESCENCE

B. Holyñska, B. Ostachowicz, J. Ostachowicz, L. Samek, D. Wegrzynek, University of Mining and Metallurgy, Kraków, Poland

10:10 Break

10:30 F-16 DECONVOLUTION OF THE INSTRUMENTAL PROFILE FUNCTION FROM SOFT Fe L X-RAY SPECTRA

G. Trudgett, R. Cheary, University of Technology, Sydney, Australia
K. Turner, BHP Steel, Australia

10:50 F-17 INTELLIGENT INTERPOLATION FOR BACKGROUND SUBTRACTION IN TRACE-ELEMENT ANALYSIS

R.A. Couture, Washington University, St. Louis, MO

11:10 F-21 NON-DESTRUCTIVE EDXRF ANALYSIS OF GARMENT BUTTONS

G.S. Hall, Rutgers University, Piscataway, NJ

11:30 F-36 BACKGROUND REMOVE IN XRF SPECTRUM – A COMPARISON OF VARIOUS TECHNIQUES

T. He, CMI International Corporation, Elk Grove Village, IL

Local Attractions*

Museums

Denver Art Museum, (303) 640-2793
Museum of Western Art, (303) 296-1880
Denver Museum of Natural History, (303) 322-7009
IMAX Theater, (303) 370-6300
Gates Planetarium, (303) 370-6351
Molly Brown House Museum, (303) 832-4092

Performing Arts

Denver Center for the Performing Arts, (303) 893-3272
Center Attractions, (303) 893-4100
Denver Center Theater Company, (303) 893-4000
Symphony Orchestra (Boettcher Concert Hall), (303) 592-7777
Temple Buell Theater, (303) 640-2862
Opera Colorado, (303) 778-6464
Paramount Theater, (303) 534-8336

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Hudson Gardens, (303) 797-8565
The Denver Zoo, (303) 331-4100
Elitch Gardens, (303) 455-4771
Coors Field, (303) 762-5437
Mile High Stadium, (303) 649-9000
Red Rocks Outdoor Amphitheater, (303) 572-4700
Fiddler's Green Outdoor Amphitheater, (303) 220-7000

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AMC Theaters, Highlands Ranch 24
C-470 & Broadway, (303) 790-4262

Mann Theaters, Tamarac Square
7777 E. Hampden, (303) 755-5100

United Artists, Continental
Hampden & I-25, (303) 758-2345

United Artists, Greenwood Plaza
8141 E. Arapahoe Road, (303) 741-1200

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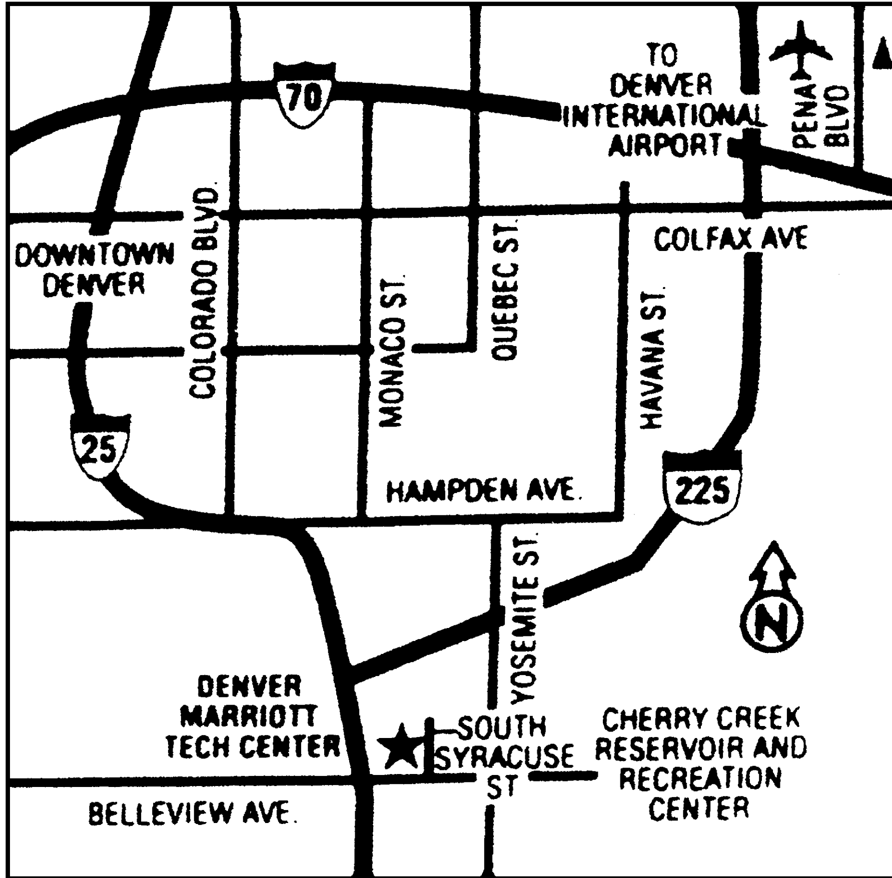
Directions to Denver Marriott Tech Center Hotel*



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From Denver International Airport: Take Peña Boulevard to I-70 West to I-225 South. From I-225 South, take Yosemite (Exit 2). Continue on Yosemite heading west along the frontage road to D T C Boulevard; turn left. Go south to East Union Avenue; turn right. Go west to South Syracuse Street; turn left. The Denver Marriott Tech Center is on the right.

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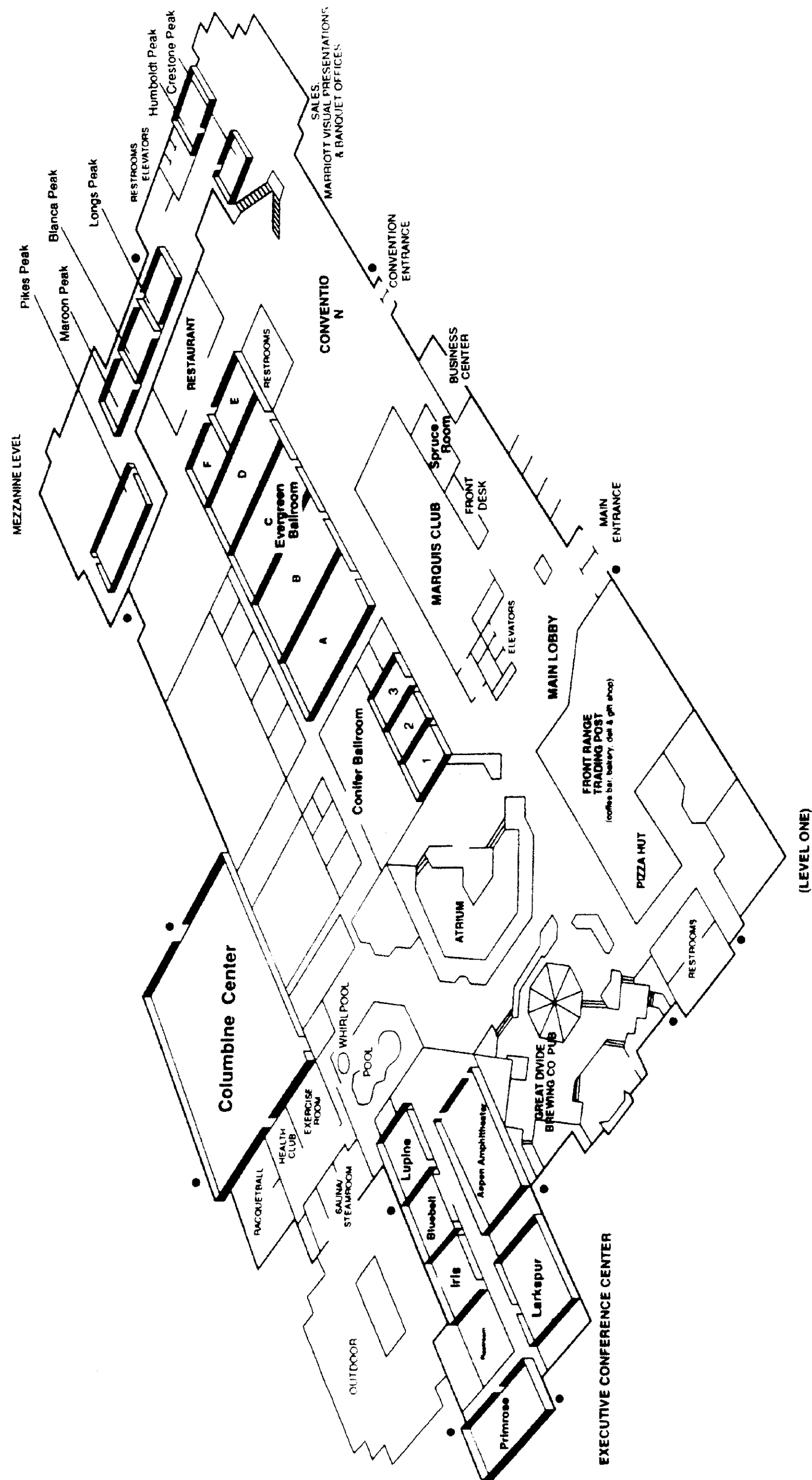
Denver Marriott Tech Center Hotel*

Hotel Layout



DENVER MARRIOTT TECH CENTER

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Program-At-A-Glance

31 July – 4 August 2000

Day & Time	XRD & XRF	XRD	XRF
Sun. eve.: 5:30–7:30 **Welcoming Reception** Sponsored by: Bede Scientific, SPEX CertiPrep & Claisse Scientifique **(Atrium)**			
MON. am: **Workshops**	**W-1** New Methods of Beam Conditioning **Faber/Bowen (A)**	**W-2** Hands On Rietveld Analysis I **Dinnebier/Antipov (B)** **W-3** Alignment & Standards **Cline/Cheary (C)**	**W-4** Practical TXRF **Zaitz/Wobrauschek/Streli (D)**
MON. pm: **Workshops**		**W-5** Hands On Rietveld Analysis II **Dinnebier/Antipov (B)** **W-6** Analysis of Micron Size Specimens **Goehner (A)**	**W-7** Introduction to XRF **Jenkins/Croke (C)** **W-8** Analysis of Layered Materials by XRF **Dirken (D)**
MON. eve.: 6:30–8:30 **Philips Analytical Reception** and **XRD Poster Session I** (Huang/Snyder) Sponsored by: Philips Analytical **(Evergreen)**			
TUE. am: **Workshops**		**W-9** Residual Stress Analysis **Noyan/Goldsmith (A)** **W-10** Phase Transformation **Jones (B)**	**W-11** Specimen Preparation XRF I **Buhrke et al (C)** **W-12** Fundamental Parameters **Mantler (D)**
TUE. pm: **Workshops**		**W-13** Grazing Incidence **Huang/Harada (B)** **W-14** Texture Analysis **De Angelis/Schaeben (D)**	**W-15** Specimen Preparation XRF II **Buhrke (C)** **W-16** Quantitative Analysis – Standardless Methods **Anzelmo (A)**
TUE. eve.: 6:30–8:30 **MDI and Rigaku/USA Reception** and **XRD Poster Session II** (O'Connor/Predecki) Sponsored by: MDI & Rigaku/USA **(Evergreen)**			
WED. am.: 8:30–12:00 noon **Plenary Session: "X-ray Analysis in the 21st Century"** (Jenkins/Predecki) **(Evergreen)**			
WED. pm: **Sessions**	**C-1** Problems & Solutions in XRD/XRF **Buhrke/Smith (A)**	**D-1** Rietveld Analysis **Dinnebier/Antipov (B)** **D-2** Mesostructure Analysis **Snyder/Barton (C)**	**F-1** Industrial Applications of XRF I **Wilson/Broton (D)**
WED. eve: 6:30 – 8:30 **Bruker AXS, Inc. Reception** and **XRF Poster Session** (van Grieken/Havrilla) Sponsored by: Bruker AXS, Inc. **(Evergreen)**			
THURS. am: **Sessions**	**C-2** Microbeam Techniques I **Ice/Noyan (E&F)**	**D-3** Stress Analysis I **Fiala/Winholtz (B)** **D-4** Phase Transformations and Reactions I **Üstündag/Bourke (C)**	**F-2** New Developments in XRF I **Buhrke/Zaitz (D)**
THURS. pm: **Sessions**	**C-3** Microbeam Techniques II **Ice/Noyan (E&F)**	**D-5** Stress Analysis II **Predecki/Sasaki (B)** **D-6** Phase Transformations and Reactions II **Üstündag /Bourke (C)** **D-7** New Developments in XRD Instrumentation I **Misture/Ungar (A)**	**F-3** New Developments in XRF II **Zaitz/Buhrke (D)**
THURS. eve.: 5:00 – 6:00 **IXAS (Conifer)** 7:00 **Conference Dinner.** (Guest Lecturer, D.K. Smith) **(Evergreen)**			
FRI. am: **Sessions**		**D-8** New Developments in XRD Instrumentation II **Misture/O'Connor (A)** **D-9** Thin films Analysis XRD **Huang/Lin/Harada (B)**	**F-4** Industrial Applications of XRF II **Baker/Havrilla (D)** **F-5** Quantitative XRF & Software **Mantler/van Grieken (C)**

Meeting Rooms are noted in parentheses: All sessions will be held in a section(s) of the Evergreen Ballroom—Sections A, B, C, D, E or F.

Any changes to program will be reflected in the *Book of Abstracts* and on the Denver X-ray Conference web page: http://www.dxcicdd.com.

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TRAVEL FORM

2000 Denver X-ray Conference Registration Form

Denver Marriott Tech Center Hotel, 31 July – 4 August 2000
Denver, Colorado, U.S.A.

Please circle the workshops that you plan to attend:

W-1 W-2 W-3 W-4 W-5 W-6 W-7 W-8 W-9 W-10 W-11 W-12 W-13 W-14 W-15 W-16

The reduced registration fee will only be applied if **registration form and payment** are received on or before 14 July 2000.

Registration Fees:	**by July 14**	**after July 14**
☐ Full week: exhibits, workshops, sessions†	$275	$325
☐ Monday & Tuesday: exhibits, workshops†	$225	$275
☐ Wed., Thurs. & Friday: exhibits, sessions†	$225	$275
☐ Session organizers, invited speakers and workshop instructors†	$100	$100
☐ Students, unemployed X-ray people, and persons 65 and older‡: full week – exhibits, workshops, sessions	$50	$50
☐ Conference dinner, Thursday evening	$30	$30

†Includes a copy of Volume 44 of ***Advances in X-ray Analysis*** on CD-ROM

‡Students and those unemployed must have their status confirmed by phone or letter to the Conference Coordinator (see information at bottom of page). Students registering at the conference are required to show I.D.

☐ ***Advances in X-ray Analysis*****,** Cumulative Volumes 1–39 on CD-ROM: $350
☐ ***Advances in X-ray Analysis*****,** Volumes 40 on CD-ROM: $150
☐ ***Advances in X-ray Analysis*****,** Volumes 41 on CD-ROM: $150
☐ ***Advances in X-ray Analysis*****,** Volumes 42 on CD-ROM: $150
☐ ***Powder Diffraction***✫(Individual one year subscription for the year 2001): Domestic $60 / Overseas $85
☐ ***Powder Diffraction***✫(Institution one year subscription for the year 2001): Worldwide $105

✫See further information regarding ***Powder Diffraction*** on page 2 of this program

Please print clearly to avoid errors on name tags and registration list.

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❑ Charge my: ❑ Visa ❑ Mastercard ❑ American Express

Card number ______________________________ Expiration date ____________

Signature ______________________________

Send registration form and payment to: ICDD, Denise Flaherty, Conference Coordinator, 12 Campus Boulevard, Newtown Square, PA 19073-3273, U.S.A. E-mail dxc@icdd.com ◆ phone 610-325-9814 ◆ fax 610-325-9823

Return by 14 July 2000

49th Annual

Denver X-ray Conference

Denver Marriott Tech Center Hotel

Denver, Colorado U.S.A.

31 July – 4 August 2000

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