Plenary Session
RED HOT X-RAYS

2–6 August 2004
Sheraton Steamboat Resort
Steamboat Springs, Colorado  U.S.A.

Sponsored by
International Centre for Diffraction Data
53rd Annual
Denver X-ray Conference

Sheraton Steamboat Resort
Steamboat Springs, Colorado U.S.A.
2-6 August 2004

2004 Denver X-ray Conference Organizing Committee

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Don Broton, Construction Technology Labs, Skokie, IL
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John V. Gilfrich, Emeritus, SFA, Inc./NRL, Bethesda, MD
George J. Havrilla, Los Alamos National Laboratory, Los Alamos, NM
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James A. Kaduk, BP Chemicals, Naperville, IL
Terry Maguire, Conference Administrator, International Centre for Diffraction Data, Newtown Square, PA
Scott T. Misture, NYS College of Ceramics at Alfred University, Alfred, NY
I. Cev Noyan, IBM, Yorktown Heights, NY
Robert L. Snyder, Georgia Institute of Technology, Atlanta, GA
Mary Ann Zaitz, IBM, Hopewell Junction, NY

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.

Front cover: image of Mount St. Helens by M.P. Doukas, July 22, 1980 courtesy of U.S. Geological Survey/Cascades Volcano Observatory
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Accommodations and Travel

Hotel Information

The 2004 Denver X-ray Conference will be held 2-6 August at the Sheraton Steamboat Resort, 2200 Village Inn Court, P.O. Box 774808, Steamboat Springs, Colorado 80477, U.S.A., phone: 1.800.848.8877 or 1.970.879.2220, fax: 1.970.879.7322, e-mail: Reservations.Steamboat@Sheraton.com, web site: http://www.steamboat-sheraton.com.

Reservations

Please identify yourself as a Denver X-ray Conference attendee when booking your reservation. Attendees are responsible for making their own reservations. Reservations should be made as soon as possible since there is a limited number of rooms available at the conference rate. Standard View rooms have been contracted at the conference rate of $109 per day plus 9.4% tax. Rates are only applicable until 25 June 2004 (subject to availability). There is an optional $8 per room per day resort fee. The Sheraton is also extending special view rooms to Denver X-ray Conference attendees at a discounted rate: Valley View rooms for $119 per day plus tax; Slope View rooms for $129 per day plus tax. Please visit the Sheraton web site: www.steamboat-sheraton.com for a description of the rooms. No shows, late arrivals and early departures will be assessed the total payment for the full length of stay as originally booked unless room is resold.

Student Rooms

There are a limited number of restricted view hotel rooms being offered to students at a discounted rate of $85 per night plus 9.4% tax. Student rooms are shared—each room will be equipped with two queen beds to accommodate two persons. Please visit the Denver X-ray Conference web site: www.dxiccdd.com for a Student Room Authorization form. Student identification will be required. Rooms will be booked on a first come first serve basis. No shows, late arrivals and early departures will be assessed the total payment for the full length of stay as originally booked unless room is resold.

Overflow Hotel

The Steamboat Grand Resort Hotel, 2300 Mt. Werner Circle, Steamboat Springs, Colorado, U.S.A. has been contracted as the overflow hotel. Please identify yourself as a Denver X-ray Conference attendee when booking your reservation.

Phone: 1.970.871.5050 or 1.877.269.2628
Fax: 1.970.871.5051
E-mail: grandbookit@steamboat.com
Web site: www.steamboatgrand.com

Studio/Parlor rooms have been contracted for $109 per night plus 14.9% tax and resort fee. Rates are only applicable until 30 June 2004 (subject to availability). A nonrefundable deposit equal to one night’s room charge will be assessed to each individual’s credit card at time of reservation.

Need a Roommate?

If you are unable to pay the full price of a hotel room, consider sharing the expenses with a roommate. Check out the Denver X-ray Conference web site: www.dxiccdd.com for information on locating a roommate.

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. A request for air travel is included on page 41 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 out of state. 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 number when making your reservations. The number is as follows:

United Airlines Phone: 1.800.241.6522 DXC Reference Number: 524AE
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 5 July 2004. The reduced registration fee will only be applied if registration form and payment are received on or before 5 July 2004.

Attendees paying by credit card, may pre-register on-line at www.dxcicdd.com. Attendees who are paying by check, or who need to verify their status as either student, unemployed or over 65, need to complete a registration form. Please go to page 43 of this Program for the registration form, or print a copy from the conference web site. After completing your form, please send 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.

Conference Registration Fees

<table>
<thead>
<tr>
<th>Service</th>
<th>Discount</th>
<th>After 5 July</th>
</tr>
</thead>
<tbody>
<tr>
<td>Full week: exhibits, workshops, sessions‡</td>
<td>$375</td>
<td>$450</td>
</tr>
<tr>
<td>Monday &amp; Tuesday: exhibits, workshops‡</td>
<td>$325</td>
<td>$400</td>
</tr>
<tr>
<td>Wednesday, Thursday &amp; Friday: exhibits, sessions‡</td>
<td>$325</td>
<td>$400</td>
</tr>
<tr>
<td>Session organizers, invited speakers &amp; workshop instructors‡</td>
<td>$100</td>
<td>$100</td>
</tr>
<tr>
<td>Students, unemployed, and persons 65 and older: exhibits, workshops, sessions</td>
<td>$75</td>
<td>$75</td>
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</tbody>
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*Preregistration fees will only be valid until 5 July 2004. Registration fees will increase after 5 July 2004.

‡Includes a copy of Volume 48 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: $380
- **Advances in X-ray Analysis**, Individual Volumes 40–46 on CD-ROM: $160 each
- **Powder Diffraction** (Individual one year subscription):
  - Domestic: Online: $80 $90 Print: $80 $90 Print & online: $100 $110
  - Overseas: Online: $80 $90 Print: $105 $115 Print & online: $130 $140
- **Powder Diffraction** (Institution one year subscription):
  - Worldwide: Online: $110 $120 Print: $155 $175 Print & online: $175 $185
  - Student online: $35

### Powder Diffraction

*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.

Web site: opis.aip.org/pdi

On-site Registration:

All on-site registrations will be conducted at the Conference Registration Desk, located on the ground floor (level one) of the Sheraton Steamboat Resort. See the hotel layout on page 38 of this program for the exact location.

Registration Times:

- Sunday, 1 August 4:00 p.m.-7:00 p.m.
- Monday, 2 August 8:00 a.m.-3:00 p.m.
- Tuesday, 3 August 8:00 a.m.-3:00 p.m.
- Wednesday, 4 August 8:00 a.m.-2:00 p.m.
- Thursday, 5 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:** Cancellations must be submitted in writing to the Conference Coordinator. A full refund will be issued, less a $50 processing fee, if the cancellation is received at least two weeks before the conference (Monday, 19 July 2004). No refunds will be issued for cancellations received after 19 July 2004.
Exhibitor Information

Exhibits will be located in the foyer, Sunset, Sunshine Peak and Mt. Werner rooms on the ground floor of the hotel. A diagram of the exhibit locations will be available in the Book of Abstracts and on the DXC web page at http://www.dxcicdd.com

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 April 2004

- AMPTEK, Inc.
- ATPS, Inc.
- Bede Scientific, Inc.
- Blake Industries, Inc.
- Bruker AXS, Inc.
- Brushwellman Electrofusion Products
- Corporation Scientifique Claisse, Inc.
- EDAX, Inc.
- Engelhard Corporation
- GBC Scientific Equipment Pty Ltd.
- Handley Analytical Services
- Inel, Inc.
- International Centre for Diffraction Data (ICDD)
- Kratos Analytical
- Laval Lab, Inc.
- LND, Inc.
- Materials Data, Inc. (MDI)
- MOXTEK, Inc.
- Osmic, Inc.
- Oxford Instruments
- PANalytical
- Premier Lab Supply
- Rigaku/MSC, Inc.
- Rocklabs Ltd.
- Spectrum Plus
- SPEX CertiPrep, Inc.
- Thales Components Corporation
- Thermo Electron
- Wiley
- Xenocs SA
- X-ray Instrumentation Associates
- X-ray Optical Systems, Inc.

All exhibitors are invited to attend the Exhibitors’ General Meeting

Wednesday, 4 August 2004, 5:30–6:00 p.m. in the Skyline Room

Note to Exhibitors:

The ceiling heights for the exhibit areas are as follows:
- Foyer—9' to light fixtures
- Sunset Room—9'4"
- Mt. Werner and Storm Peak Room—14'6"
Evening Technical Sessions and Social Functions

Spouses are welcome to attend all social functions.
Location of Evening Mixers and Poster Sessions will be announced at the Conference.

Sun., 1 August  6:00–8:00  Welcoming Reception
                Sponsored by Corporation Scientifique Claisse, SPEX CertiPrep
                and Wiley

Mon., 2 August  6:00–8:00  XRD Poster Session I
                Sponsors to be announced

Tues., 3 August  6:00–8:00  MDI and Rigaku/MSC, Inc. Reception & XRD Poster Session II
                Sponsored by Materials Data, Inc. and Rigaku/MSC, Inc.

Wed., 4 August  6:00–8:00  Bruker AXS, Inc. Reception & XRF Poster Session
                Sponsored by Bruker AXS, Inc.

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 Daybreak room from 9:30 to 10:30 a.m. on
Monday and Tuesday. Information on local attractions and activities of interest will be provided.

General Information

Poster Boards
The poster boards used during the evening poster sessions will be 4’ x 6’ boards. Authors must bring
their own thumbtacks or Velcro.

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
The DXC Book of Abstracts will be available at the Conference Registration Desk.
examined. Discussions will include quantifying the quality of the results, graphical results and several statistical tools used to judge the quality of the fit between theory and experiment.

The major components of this workshop are on problem solving and the identification of needs for improved experimental or modeling methods. Problems that can be assigned to either data quality or deficiencies of the refinement model will be identified. Methods to overcome these problems will be explored.

W-3 Specimen Preparation XRF I Skyline

Organized by:
J.A. ANZELMO, Anzelmo & Associates, Madison, WI
D. BROTON, Construction Technology Labs, Skokie, IL

Instructors:
D. BROTON, Construction Technology Labs, Skokie, IL
R. BOSTWICK, SPEX CertiPrep Inc., Metuchen, NJ
L. CREAMER, Timet, Morgantown, PA

J. PETRE, Corporation Scientifique Claisse, Inc., Sainte-Foy (Quebec), Canada

This workshop covers the basics and specific details of sampling and specimen preparation for a wide variety of materials. Novel approaches to preparing specimens for analysis come from instructors with many years of experience applying various techniques to real-world samples. Whether an analyst is new to X-ray techniques or experienced, the workshop provides both broad topics and specialized techniques developed for a specific analytical goal.

W-4 Thin Film XRF Analysis Twilight

Organized by:
M. DIRKEN, PANalytical, Almelo, The Netherlands

Instructors:
M. DIRKEN, PANalytical, Almelo, The Netherlands
A. WITKOPP, Thermo NORAN, Middleton, WI

J. AVERITT, PANalytical, Inc., Tempe, AZ

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. This is highlighted by ED-XRF and WD-XRF examples focusing on practical issues including problems of finite thickness and line selection.
### W-5 X-ray Physics Rainbow

**Organized by:**
W.T. Elam, University of Washington, Seattle, WA

**Instructors:**
W.T. Elam, University of Washington, Seattle, WA
T. Jach, National Institute of Standards & Technology, Gaithersburg, MD
B. Ravel, Naval Research Laboratory, Washington, DC

The X-ray Physics workshop will start with a description of the interactions of X-rays with atoms. These will then be used to develop the physics of X-ray measurements of materials, which are collections of atoms. Topics to be covered include XRD, XRF, XAFS, TXRF, and detector physics (including superconducting detectors). It is our intention that at least half of the material will be useful to anyone with a technical Bachelor's degree, with the remainder aimed at the PhD level.

### W-6 Optics Twilight

**Organized by:**
S.T. Misruise, NYS College of Ceramics at Alfred University, Alfred, NY
G.J. Havilla, Los Alamos National Laboratory, Los Alamos, NM

**Instructors:**
D.K. Bowen, Bede Scientific Inc., Englewood, CO
D. Gibson, X-ray Optical Systems, Inc., East Greenbush, NY
L. Jiang, Osmic, Inc., Auburn Hills, MI
P. Dinh, Horiba Instruments, Inc., Irvine, CA

There are a myriad of X-ray optics on the market and each one has its own unique capabilities in terms of X-ray spectrometry. This workshop will provide the basic knowledge about X-ray optics including: multilayer optics, crystal optics, polycapillary optics and moncapillary optics. One objective is to help users understand the basic working principles and performance characteristics of these optics. Attendees will learn the function of an optical system in an X-ray instrument. Applications of these optics and their capabilities will be presented.

### W-7 Rietveld Applications II Storm Peak

**Organized by:**
A. Kern, Bruker AXS GmbH, Karlsruhe, Germany
J. Faber, International Centre for Diffraction Data, Newtown Square, PA

Continuation of W-2 Rietveld Applications I.

### W-8 Specimen Preparation XRF II Skyline

**Organized by:**
J.A. Anzelmo, Anzelmo & Associates, Madison, WI
D. Broton, Construction Technology Labs, Skokie, IL
R. Bostwick, SPEX CertiPrep Inc., Metuchen, NJ
L. Creasy, Timet, Morgantown, PA
J. Pitre, Corporation Scientifique Claisse, Inc., Sainte-Foy (Quebec), Canada

Continuation of W-3 Specimen Preparation XRF I.
W-9  Microbeam X-ray Stress Analysis
Rainbow
Organized by:
I.C. NOYAN, IBM, Yorktown Heights, NY
Instructors:
I.C. NOYAN, IBM, Yorktown Heights, NY
N. TAMURA, Lawrence Berkeley National Laboratory, Berkeley, CA
This workshop is designed to introduce the attendees to the measurement of applied and residual stresses using X-ray diffraction. Both theoretical fundamentals and practical aspects of the measurement will be discussed, including basic stress analysis theory and its extensions to microbeam systems including white beam, pink beam and monochromatic techniques, measurement volume considerations, instrument stability, focusing optics, and dedicated synchrotron instruments for stress measurements.

W-10 Total Pattern Analysis (TPA)
Storm Peak
Organized by:
J. FABER, International Centre for Diffraction Data, Newtown Square, PA
T. FAWCETT, International Centre for Diffraction Data, Newtown Square, PA
R.L. SNYDER, Georgia Institute of Technology, Atlanta, GA
Instructors to be announced
Qualitative and quantitative phase analyses have always rested with the description of diffraction results in terms of a concise peak-list, i.e., d-spacing/peak intensity pairs. However, there are obvious short-comings in this approach. Important details concerning background variations, amorphous components in the scattering pattern, peak-width and instrumental resolution have been removed from consideration. In the first part of this workshop, we will show qualitatively how these short-comings affect the quality of pattern matching using selected examples from PDF-4 Relational Databases. In the second part of this workshop we will examine methods for TPA and explore how TPA aids in the recovery of search-indexing details that have been overlooked or lost.

W-11 Quantitative XRF I
Twilight
Organized by:
M. MANTLER, Vienna University of Technology, Vienna, Austria
Instructors:
M. MANTLER, Vienna University of Technology, Vienna, Austria
B. VREBOO, PANalytical, Almelo, The Netherlands
W.T. ELAM, University of Washington, Seattle, WA
Part 1:
• Fundamentals
• Classical fundamental parameter models and mathematical foundation
• Computed (theoretical) influence coefficients and their mathematical relationship to fundamental parameter models
• Compensation methods
• Error analysis and error propagation, iteration schemes, determination of elements by difference
Part 2:
Selected special cases and methods. This year the focus will be placed on Monte Carlo methods:
• Mathematical and statistical principles
• Applications: Irregularly shaped specimens, inhomogeneous specimens, micro-XRF; unusual geometrical situations
• What means “quantitative analysis” with inhomogeneous specimens?
• Practical aspects: Accuracy and computing times

W-12 Fundamentals of XRF
Skyline
Organized by:
L. CREASY, Timet North American Operation, Morgantown, PA
Instructors:
L. CREASY, Timet North American Operation, Morgantown, PA
J. SIEBER, National Institute of Standards & Technology, Gaithersburg, MD
M. KROC, Minerals Technology, Easton, PA
This workshop is intended to provide a basic background of the principles of XRF, specifically directed to those new to the field. It will consist of a general overview of the technique, followed by more specific details of particular applications by experts in those applications, to provide an understanding of the use of the principles previously described.
**XRD & XRF**

**W-13 Principles and Use of Micro-diffraction & Microfluorescence**

**Rainbow**

*Organized by:*

T.N. Blanton, Eastman Kodak Company, Rochester, NY

*Instructors:*

T.N. Blanton, Eastman Kodak Company, Rochester, NY

R.P. Goehner, Sandia National Laboratories, Albuquerque, NM

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

B.B. He, Bruker AXS, Inc., Madison, WI

This workshop will cover characterization of materials using micro X-ray diffraction, micro X-ray fluorescence, and electron backscattered diffraction techniques. The instructors will cover why one would use micro techniques, the equipment, experimental procedures used to perform data collection, analysis of data, and examples of how these micro analysis methods have been used to solve materials problems.

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**W14 Specimen Preparation—XRD**

**Skyline**

*Organized by:*

T. Fawcett, International Centre for Diffraction Data, Newtown Square, PA

*Instructors:*

M. Rodriguez, Sandia National Laboratories, Albuquerque, NM

G. Stephenson, Eli Lilly and Company, Indianapolis, IN

T. Fawcett, International Centre for Diffraction Data, Newtown Square, PA

Specimen preparation is often the limiting step for obtaining good results in any diffraction experiment. Preparation methods can influence the precision and accuracy of peak positions, intensities, and intensity profiles, the basic measurements required for qualitative and quantitative analyses. The presentation will focus on crystallite and particle effects, orientation and texture, and how they influence the resulting data and what steps can be taken to reduce or eliminate these influences. Preparation techniques for different instrumentation and sample holders will be covered and examples will be given for a wide range of materials such as minerals, metals and pharmaceuticals. Tricks of the trade taken from the literature and global X-ray community will be discussed.

**W-15 Small Angle Scattering**

**Storm Peak**

*Organized by:*

N.S. Murthy, University of Vermont, Burlington, VT

J.D. Londono, DuPont Company, Wilmington, DE

*Instructors:*

R. Hjelm, Los Alamos National Laboratory, Los Alamos, NM

P. Jemian, UNICAT at Advanced Photon Source, Argonne National Laboratory, Argonne, IL

B. Hsiao, SUNY, Stony Brook, NY

Small-angle scattering provides structural information on length scales of 1 to 100 nm. Typical applications include characterization of particles (colloids, proteins and polymers in solution), pore size analysis (ceramics, metals and polymers), and nanostructures such as lamellae in semicrystalline polymers. The workshop will introduce new users to the instrumentation, data analysis and interpretation while providing a sufficiently broad overview for experienced users to identify new opportunities in three areas: 1) Neutron scattering and its application to polymers and proteins. 2) X-ray scattering including ultra-small angle X-ray scattering with examples from ceramics. 3) In situ X-ray scattering using synchrotron radiation for studying crystallization and fiber formation in polymers. The three sections of the workshop will be given by three experienced instructors who, with their different approaches, will give a broad overview of the entire field.

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**XRF**

**W-16 Quantitative XRF II**

**Twilight**

*Organized by:*

M. Mantler, Vienna University of Technology, Vienna, Austria

*Instructors:*

M. Mantler, Vienna University of Technology, Vienna, Austria

B. Vrebos, PANalytical, Almelo, The Netherlands

W.T. Elam, University of Washington, Seattle, WA

Continuation of W-11 Quantitative XRF I.
Poster Sessions:
Monday, 2 August–Wednesday, 4 August
6:00–8:00 p.m.

Poster Boards
The poster boards used during the evening poster sessions will be 4’ x 6’ boards.
Authors must bring their own thumbtacks or Velcro.

*Held in conjunction with evening receptions*

Oral Sessions:
Wednesday, 4 August–Friday, 6 August
Times vary

*Please consult the Program for exact times*
The XRD Poster Session I will be held in conjunction with the evening mixer. Sponsors to be announced.

**Chairs:** R.L. Snyder, Georgia Institute of Technology, Atlanta, GA  
J.A. Kaduk, BP Chemicals, Naperville, IL

*Session chairs will select the two best papers for awards.*

**Stress**

**C-1 STUDY OF DYNAMIC AND STATIC STATES OF SHOCK WAVES INDUCED DEFORMATION**  
F.A. Selim, D.P. Wells, J.F. Harmon, J.R. Williams, *Idaho State University, Pocatello, ID*

**D-073 X-RAY DIFFRACTION STUDIES OF ZnO NANOCAGES**  
I. Dragomir-Cernatescu, P.X. Gao, Z.L. Wang, R.L. Snyder, *Georgia Institute of Technology, Atlanta, GA*

**D-087 ELASTIC PROPERTIES AND LAMELLAR STRUCTURE OF TiAl SYSTEM INTERMETALLIC COMPOUNDS**  
H. Hirose, Kinjo University Research Center, Ishikawa, Japan  
T. Murotani, Dalian University, Dalian Economic and Technical Development Zone, China  
M. Gotoh, Kanazawa University, Ishikawa, Japan  
H. Tabata, Industrial Research Institute of Ishikawa, Ishikawa, Japan

**D-085 SCRATCH TEST OF THIN FILMS HAVING RESIDUAL STRESS AND FIBER TEXTURE**  
M. Gotoh, T. Sasaki, Y. Hirose, Kanazawa University, Ishikawa, Japan

**D-086 X-RAY STRESS MEASUREMENT OF GROUND SURFACE OF DENTAL MATERIAL**  
C. Zhou, M. Gotoh, Kanazawa University, Ishikawa, Japan  
H. Hirose, Kinjo University, Ishikawa, Japan  
M. Shozu, Maizuru National College of Technology, Kyoto, Japan

**D-079 LARGE SPECIMEN X-RAY AND NEUTRON DIFFRACTION RESIDUAL STRESS FACILITIES**  
C.R. Hubbard, T.R. Watkins, M.C. Wright, A.D. Stoica, W.B. Bailey, *Oak Ridge National Laboratory, Oak Ridge, TN*

**D-078 RESIDUAL STRESS MEASUREMENTS OF CAST ALUMINUM ENGINE BLOCKS USING X-RAY DIFFRACTION**  
D.J. Wiesner, University of Tennessee, Knoxville, TN  
J.C. Williams, Ohio State University, Columbus, OH

**D-055 MATERIAL EVALUATION OF RAILS BY X-RAY STRESS MEASUREMENT**  
T. Sasaki, Y. Kanematsu, Y. Hirose, Kanazawa University, Kanazawa, Japan  
Y. Sato, K. Iwafuchi, Railway Technical Research Institute, Tokyo, Japan  
K. Hiratsuka, Kyushu Polytechnic University, Fukuoka, Japan  
T. Yamane, Fuji Photo Film Co., Ltd., Tokyo, Japan
XRD Poster Session I—Monday, 2 August
6:00 p.m.–8:00 p.m.

D-054  EFFECT OF MICROCRACKS AND RESIDUAL STRESS OF Cr PLATING LAYER ON FATIGUE STRENGTH
Y. Kobayashi, J. Nagasawa, Tokico Ltd., Kawasaki, Japan
Y. Kanematsu, T. Sasaki, Y. Hirose, Kanazawa University, Kanazawa, Japan

D-043  RESIDUAL STRESS IN UNI-DIRECTIONALLY DEFORMED SURFACE LAYER BY SHOTPEENING ON SPRING STEEL
T. Sakakibara, Chuo Spring Co., Ltd., Japan
Y. Sato, Osaka City University, Japan

D-038  COMPLEX DESCRIPTION OF SUBSTRUCTURE, RESIDUAL STRAIN AND LATTICE DEFECTS IN TEXTURED METAL MATERIALS BY USE OF GENERALIZED POLE FIGURES
Yu. Perlovich, M. Isaenko, Moscow Engineering Physics Institute (State University), Moscow, Russia

D-028  ANALYSIS OF RESIDUAL STRESS STATE OF HARDMETAL CARBIDE CUTTING TOOL SUBSTRATES
M.F. Beclo, Kennametal Inc., Latrobe, PA

D-025  RESIDUAL STRESSES AND SIZE-STRAIN PHENOMENA IN THERMALLY CYCLED Cu LAYERS ON ANISOTROPICAL SiO₂(110) SUBSTRATES
E. Eiper, M. Hafok, J. Keckes, Erich Schmid Institute, Austrian Academy of Sciences and University Leoben, Austria
C. Eisenmenger-Sittner, Vienna University of Technology, Vienna, Austria

Rietveld

D-088  STRUCTURAL INVESTIGATION OF (Ba1-xSrₓ)₂TiO₄ USING SYNCHROTRON AND LABORATORY X-RAY
J.A. Kaduk, BP Chemicals, Naperville, IL
W. Wong-Ng, J. Frank, National Institute of Standards and Technology, Gaithersburg, MD

D-093  FULL-PATTERN CLUSTER ANALYSIS ON X-RAY POWDER DIFFRACTION DATA
T. Degen, PANalytical, Almelo, The Netherlands

D-080  LONG-RANGE AND SHORT-RANGE ORDERING IN Y-DOPED La₂Zr₂O₇
T.E. Proffen, Los Alamos National Laboratory, Los Alamos, NM

D-042  ON THE FORMATION OF BROWNMLERITE AND THE CHOICE OF STRUCTURE ON THE ACCURACY OF THE RIETVELD METHOD
S.Y. Nelson, C. Mattern, R.S. Winburn, Minot State University, Minot, ND

D-002  RIETVELD PROCESSING OF PHASES IN HIGHLY TEXTURED REFRACTORY STEELS
J.L. Garin, R.L. Mannheim, Universidad de Santiago de Chile, Santiago, Chile
The XRD Poster Session II will be held in conjunction with the MDI and Rigaku mixer

<table>
<thead>
<tr>
<th>Session</th>
<th>Title</th>
<th>Authors</th>
<th>Institution</th>
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<tr>
<td>D-094</td>
<td>IN SITU X-RAY INVESTIGATIONS ON DIFFERENT DEHYDRATION STAGES OF</td>
<td>U. König, H. Pöllmann</td>
<td>University of Halle, Halle, Germany</td>
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<td>MANGANESE-LAYERED DOUBLE HYDROXIDES</td>
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<td>D-039</td>
<td>REACTION SEQUENCE AND KINETICS ANALYSIS FOR SYNTHESIS OF BULK Bi₄Ti₃O₁₂</td>
<td>E. Henriques, M. Haluska, M. Dolan, M.S. Peterson, S.T. Misture</td>
<td>NYS College of Ceramics at Alfred University, Alfred, NY</td>
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<td>D-033</td>
<td>HIGH TEMPERATURE X-RAY DIFFRACTION AND ELECTRON MICROSCOPY OF</td>
<td>M.S. Haluska, S.T. Misture</td>
<td>NYS College of Ceramics at Alfred University, Alfred, NY</td>
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<td></td>
<td>Bi₂Sr₂Nb₂GaO₁₁.₅</td>
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<td>D-027</td>
<td>HIGH TEMPERATURE IN SITU X-RAY DIFFRACTION OF THE SiO₂-Mg DIATOM</td>
<td>M.S. Haluska, K. Sandhiage, R.L. Snyder, S.T. Misture</td>
<td>Georgia Institute of Technology, Atlanta, GA</td>
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<td>DISPLACEMENT REACTION</td>
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<td>S.T. Misture, NYS College of Ceramics at</td>
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<td>Alfred University, Alfred, NY</td>
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<td>D-060</td>
<td>TEMPERATURE CALIBRATION FOR HIGH-TEMPERATURE X-RAY DIFFRACTION</td>
<td>M.D. Dolan, S.I. Zdzieszynski, S.T. Misture</td>
<td>NYS College of Ceramics at Alfred University, Alfred, NY</td>
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<td></td>
<td>SYSTEM FOR HIGH-TEMPERATURE PROTON CONDUCTOR DEVELOPMENT</td>
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<td>Oak Ridge, TN</td>
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<td>D-024</td>
<td>XRD INVESTIGATION OF CHEMICALLY DEACTIVATED AUTOMOBILE CATALYTIC</td>
<td>M.H. Rossouw, J. Tshilongo, W.A. Jordaan</td>
<td>National Metrology Laboratory, CSIR, Pretoria, South Africa</td>
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<td>D-046</td>
<td>INVESTIGATION OF THE MICRO STRUCTURE OF ENERGETIC CRYSTALS BY</td>
<td>M. Herrmann, Fraunhofer Institut für Chemische Technologie, Pfinztal,</td>
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<td>MEANS OF X-RAY POWDER DIFFRACTION</td>
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<td>Germany</td>
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<td>D-051</td>
<td>EXPERIMENTAL EVALUATION OF THE TEMPERATURE ACCURACY OF THE</td>
<td>M. Fransen, J. Vasterink</td>
<td>PANalytical, Almelo, The Netherlands</td>
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<td>OXFORD PHENIX CRYOSTAT—A COOL JOB</td>
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<td>D-018</td>
<td>HIGH TEMPERATURE PHASE TRANSFORMATIONS IN RARE EARTH TITANATES</td>
<td>K. Jurkschat, P. Sarin, W.M. Kriven</td>
<td>University of Illinois at Urbana-Champaign, Urbana, IL</td>
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<td>D-092</td>
<td>AN IN SITU HIGH-TEMPERATURE X-RAY DIFFRACTION STUDY OF PHASE</td>
<td>T.N. Blanton, Eastman Kodak Company, Rochester, NY</td>
<td>NYS College of Ceramics at Alfred University, Alfred, NY</td>
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<td>TRANSFORMATIONS IN SILVER BEHENATE</td>
<td>S. Misture, S. Zdzieszynski, M. Nicholas</td>
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**Instrumentation**

**D-066** STRUCTURE DETAILS OF POLYMORPHISM IN ORGANIC LIGHT EMITTING DIODE (OLED) MATERIAL, Alq₃
M. Rajeswaran, T.N. Blanton, *Eastman Kodak Company, Rochester, NY*

**D-069** STUDY OF THE PS5 CONDENSATE THIN FILMS BY THE SAXS METHOD
L. Skatkov, PCB, Israel
P. Cheremskoy, E. Sobol, O. Sobol, A. Panikarsky, V. Gomozov, *Kharkov Technical University, Ukraine*

**D-014** METHANESULFONATEHYDRATES – SYNTHESIS AND XRD INVESTIGATIONS
H. Pöllmann, S. Stöber, M. Tewelde, C. Wagner, K. Merzweiler, *University of Halle, Germany*

**D-016** THE COMPARISATION OF QUANTITATIVE XRD, OPTICAL MICROSCOPY AND CATHODOLUMINESCENCE TECHNIQUE ON ORDINARY PORTLAND CEMENT CLINKERS
N. Winkler, H. Pöllmann, *University of Halle, Germany*
J. Göse, Center for Materials Analysis, Lauf a. d. Pegnitz, Germany

**D-036** PROBING POLY(ESTER URETHANE) STRUCTURE WITH ASAXS
C.F. Welch, R.P. Hjelm, E.B. Orler, D.A. Wroblieski, M.E. Hawley, J.T. Mang, *Los Alamos National Laboratory, Los Alamos, NM*
J.B. Kortright, Lawrence Berkeley National Laboratory, Berkeley, CA

**D-072** VIBRATING SAMPLE HOLDER FOR XRD ANALYSIS WITH MINIMAL SAMPLE PREPARATION
P. Sarrazin, Apparati Inc., Mountain View, CA
S. Chipera, D. Vaniman, Los Alamos National Laboratory, Los Alamos, NM
D. Bish, Indiana University, Bloomington, IN
D. Blake, NASA Ames Research Center, Moffett Field, CA

**D-045** ETCHING METHODS FOR IMPROVING SURFACE IMPERFECTIONS OF DIAMONDS USED FOR X-RAY MONOCHROMATORS
J.A. Maj, A.T. Macrander, S.F. Kransnicki, Y. Zhong, R. Khachatryan, G.J. Waldschmidt, Y.S. Chu, Argonne National Laboratory, Argonne, IL

**D-010** 11-BM, A DEDICATED HIGH-RESOLUTION POWDER DIFFRACTION BEAMLINE AT THE ADVANCED PHOTON SOURCE

**D-044** HIGH-RESOLUTION X-RAY TOPOGRAPHY APPARATUS USING A LINE-FOCUS HYBRID MONOCHROMATOR
D.E. McCready, M.B. Toloczko, *Pacific Northwest National Laboratory, Richland, WA*

**D-082** VERY LOW ANGLE OR LARGE D-SPACING WORK USING A PLANAR X-RAY WAVEGUIDE RESONATOR AS A PRIMARY COLLIMATOR ON A CONVENTIONAL POWDER X-RAY DIFFRACTOMETER
R. Clapp, *GBC Scientific Equipment Pty Ltd., Melbourne, Australia*
The XRF Poster Session will be held in conjunction with the Bruker AXS, Inc. mixer.

Chairs: J.A. Anzelmo, Anzelmo & Associates, Madison, WI
       M.A. Zaitz, IBM, Hopewell Junction, NY

Session chairs will select the three best papers for awards.

Instrumentation

C-2 NONDESTRUCTIVE TESTING OF MOISTURE DISTRIBUTION IN WOOD USING PULSED NEUTRON SOURCE
M.A. Reda, J.F. Harmon, Idaho State University, Pocatello, ID

F-08 EVALUATION OF LOCAL SHORT-RANGE ORDER AROUND Fe ATOMS IN FePt FILMS BY X-RAY FLUORESCENCE HOLOGRAPHY
Y. Takahashi, K. Hayashi, E. Matsubara, T. Shima, K. Takanashi, Tohoku University, Sendai, Japan

F-21 COST-EFFECTIVE PROBLEM SOLVING USING PORTABLE XRF

F-22 WAVEGUIDE-RESONATOR APPLICATION FOR DIRECT X-RAY FLUORESCENCE ANALYSIS OF GAS MIXTURES
V.K. Egorov, E.V. Egorov, T.V. Bil’chic, IPMT RAS, Moscow, Russia

F-29 THIN BERYLLIUM WINDOW WITH HIGH-TEMPERATURE COMPATIBILITY
M.C. Roberts, E.C. Anderson, R. Stillwell, MOXTEK, Inc., Orem, UT

F-44 PRECIOUS METALS USE AND CARE IN SAMPLE PREPARATION
C. Fiorica, Engelhard Corporation, Carteret, NJ

F-39 A NEW SETUP FOR SYNCHROTRON RADIATION INDUCED TXRF AT HASYLAB, BEAMLINE L FOR ULTRA TRACE ANALYSIS USING A SILICON DRIFT DETECTOR
C. Streli, P. Wobrauschek, C. Jokubonis, Atominstiitut, Vienna University of Technology, Wien, Austria
G. Peponi, ITC-irst, Trento, Italy
G. Falkenberg, HASYLAB at DESY, Hamburg, Germany
G. Zaray, EÖTVOS University, Budapest, Hungary

F-48 LIGHT ELEMENT DISTRIBUTION BY A POLYCAPILLARY LENSE AND AN UTW SDD DETECTOR INSIDE A VACUUM CHAMBER
B. Frank, P. Wobrauschek, N. Zoeger, C. Streli, Atominstiitut, Vienna University of Technology, Wien, Austria

Applications

F-34 FLUORESCENCE EXCITATION OF Pb Kα RADIATION AND BACKGROUND FROM SCATTERED PRIMARY RADIATION: RESULTS FROM EXPERIMENTS AT HASYLAB AND FROM THEORETICAL MODELS
M. Mantler, P. Wobrauschek, N. Zoeger, G. Peponi, C. Streli, Vienna University of Technology, Vienna, Austria
G. Falkenberg, HASYLAB at DESY, Hamburg, Germany
XRF Poster Session—Wednesday, 4 August
6:00 p.m.—8:00 p.m.

F-37  CHARACTERIZATION OF SEDIMENTS IN NORTHEAST-HUNGARIAN RIVERS USING SINGLE-PARTICLE X-RAY EMISSION AND ABSORPTION METHODS
J. Osán, S. Török, S. Kurunczi, A. Alsecz, KFKI Atomic Energy Research Institute, Budapest, Hungary
G. Falkenberg, HASYLAB at DESY, Hamburg, Germany
R. Van Grieben, University of Antwerp, Antwerp, Belgium

F-40  COMPARISON OF RESPONSE FUNCTION FITTING WITH QXAS-AXIL NON LINEAR LEAST SQUARE FITTING- SPECTRA EVALUATION OF LOW Z ELEMENTS
H. Kaldarar, C. Streli, Atominsttitut, Vienna University of Technology, Wien, Austria

F-49  3D SR μ-XRF ON HUMAN BONE SAMPLES
N. Zoeger, P. Wobrauschek, C. Streli, Atominsttitut, Vienna University of Technology, Vienna, Austria
E. Chinea-Cano, D. Wegrzyn, Agency’s Laboratories Seibersdorf, IAEA, Vienna, Austria
P. Roschger, Ludwig Boltmann-Institut für Osteologie, Vienna, Austria
R. Simon, S. Staub, Institut für Synchrotronstrahlung, Karlsruhe, Germany
G. Falkenberg, HASYLAB at DESY, Hamburg, Germany

F-51  ELEMENTAL MAPPING OF HUMAN BRAIN BY SR-μXRF
N. Zoeger, C. Streli, P. Wobrauschek, C. Jokubonis, Atominsttitut, Vienna University of Technology, Vienna, Austria
G. Pepponi, ITC-irst, Trento, Italy
P. Roschger, Ludwig Boltmann-Institut für Osteologie, Vienna, Austria
S. Bohic, ESRF, Grenoble, France
W. Osterode, Universitätsklinik für Innere Medizin IV, Vienna, Austria

F-53  CHEMICAL-PHYSICAL CHARACTERISATION OF POLLEN WITH TXRF AND TOF-SIMS
G. Pepponi, P. Lazzeri, ITC-irst, Trento, Italy
E. Gottardini, F. Cristofolini, F. Corradini, IASMA, Trento, Italy
G. Clauser, APPA, Trento, Italy
A. Torboli, Ital Structures, Riva del Garda, Italy

F-54  GI-XRF, SIMS, MEIS: COMPLEMENTARY TECHNIQUES FOR THE CHARACTERISATION OF ARSENIC ULTRA SHALLOW JUNCTIONS
G. Pepponi, D. Giubertoni, M. Barozzi, M. Bersani, ITC-irst, Trento, Italy
N. Zoeger, C. Streli, Atominsttitut, Vienna University of Technology, Vienna, Austria
M. Werner, J.A. van den Berg, University of Salford, Salford, UK

F-03  COMBINATORIAL DEVELOPMENT OF SPECIFIC RECEPTORS FOR RADIONUCLIDE DECONTAMINATION USING MICRO X-RAY FLUORESCENCE
T.C. Miller, X-ray Optical Systems, Inc., East Greenbush, NY
M.L. Stanton, G.J. Havrilla, B.P. Warner, C.A. Wells, Los Alamos National Laboratory, Los Alamos, NM

F-16  A COMPARISON BETWEEN RIGAKU AND UNIQUANT QUANTITATIVE AND SEMI QUANTITATIVE SOFTWARE Routines
D.M. Missimer, A.R. Jurgensen, R.L. Rutherford, Westinghouse Savannah River Site, Aiken, SC

F-24  THE X-RAY FLUORESCENCE ANALYSIS OF CHLORINE IN PALLADIUM MATERIALS
A.R. Jurgensen, D.M. Missimer, R.L. Rutherford, Westinghouse Savannah River Site, Aiken, SC
F-33 RAPID EDXRF TECHNIQUES FOR MATERIALS TESTING
   S.J. Goldstein, T.M. Ellis, S.M. Trujillo, L.B. Davenhall, L.D. Sivils, Los Alamos National Laboratory,
   Los Alamos, NM

F-43 SULFUR ANALYSIS IN FUELS, A NEW APPROACH USING MONOCHROMATIC
   WAVELENGTH DISPERSIVE X-RAY FLUORESCENCE (MWD XRF)
   B. Beumer, Z. Chen, F. Wei, I. Radley, X-ray Optical Systems, Inc., East Greenbush, NY

F-52 IDENTIFICATION OF CONTAMINATIONS ON WAFERS BY X-RAY FLUORESCENCE
   TECHNIQUE
   S. Maco, K. Taniguchi, Osaka Electro-Communication University, Osaka, Japan
   T. Kurosawa, K. Aikoh, I. Hourai, Hitachi Electronics Engineering Co., Ltd, Kanagawa, Japan
**Plenary Session**

Wednesday 4 August 8:30 a.m.–12:20 p.m.

**Plenary Session: Red Hot X-rays**

Steamboat Grand Hotel

Organized by: Charles Prewitt, University of Arizona, Tucson, AZ
Robert L. Snyder, Georgia Institute of Technology, Atlanta, GA

8:30 Welcoming Remarks
Victor E. Buhke, Chairman, Denver X-ray Conference, Consultant, Portola Valley, CA

8:35 Presentation of Awards

- 2004 Birks Award presented to Tomoya Arai, Rigaku Industrial Corporation, Osaka, Japan  
  *presented by Michael Mantler*, Vienna University of Technology, Vienna, Austria
- 2004 Jerome B. Cohen Student Award (winner announced at the plenary session)  
  *presented by L. Cev Noyan*, IBM T.J. Watson Research Center, Yorktown Heights, NY
- 2004 McMurdie Award presented to Winnie Wong-Ng, National Institute of Standards & Technology, Gaithersburg, MD  
  *presented by Camden R. Hubbard*, Oak Ridge National Laboratory, Oak Ridge, TN
- 2004 Hanawalt Award presented to Robert L. Snyder, Georgia Institute of Technology, Atlanta, GA  
  *presented by James A. Kaduk*, BP Chemicals, Naperville, IL

8:55 **Hanawalt Award Lecture: The Evolution of Total Pattern Analysis**  
R.L. Snyder, Georgia Institute of Technology, Atlanta, GA

9:10 Plenary Session Remarks  
Charles Prewitt, University of Arizona, Tucson, AZ  
Robert L. Snyder, Georgia Institute of Technology, Atlanta, GA

The following are the invited papers to be presented during the plenary session:

9:15 D-95 **Getting the Hot Structures**  
K.F. Kelton, Department of Physics, Washington University, St. Louis, MO

9:55 D-7 **The Structure of Liquid Al Alloys at High Superheats Using High Energy X-Rays**  
M.J. Kramer, Ames Laboratory, Iowa State University, Ames, IA

10:35 Break

11:00 D-102 **Diffraction Studies of Order-Disorder at High Pressures and Temperatures: Transitions in Dolomite and Anhydrite**  
J.B. Parise, Geosciences, State University of NY, Stony Brook, NY

11:40 D-115 **Laue Microdiffraction for Structure Analysis at Ultra High Pressure (LAMSA UHP)—An Old Solution to a New Problem**  
P. Dera, Carnegie Institution of Washington, Geophysical Lab, Washington, DC
**PLenary Session**

Wednesday 4 August 8:30 a.m.–12:20 p.m.

**Plenary Session: Red Hot X-rays**

Steamboat Grand Hotel

**Directions to the Plenary Session:**
The Plenary Session will be held at the Steamboat Grand Resort & Conference Center Hotel, located across Mt. Werner Circle at:

- 2300 Mt. Werner Circle
- Steamboat Springs, CO 80487
- Phone: 970-871-5540
- Fax: 970-871-5541
- Web Address: www.steamboatgrand.com

The Plenary Session will be held in the Priest Creek Ballroom, located on the west side of the hotel. As you enter the hotel, proceed up a small flight of stairs to the front desk; turn right. Follow this hallway; the Priest Creek Ballroom is located near the end of it.
### SPECIAL SESSIONS

**Wednesday p.m.**

**Session C-1 \* New Developments in XRD & XRF Instrumentation**

Organized by: J.A. ANZELMO, Anzelmo & Associates, Madison, WI

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<td>1:30</td>
<td>F-42</td>
<td>ADVANCES IN THERMOELECTRICALLY COOLED SI-PIN X-RAY DETECTORS</td>
<td>A. Huber, J. Pantazis, R. Redus, T. Pantazis, Amptek, Inc., Bedford, MA</td>
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<td>1:50</td>
<td>C-5</td>
<td>MINIATURE X-RAY TUBES UTILIZING CARBON NANOTUBE-BASED COLD CATHODES</td>
<td>A. Reyes-Mena, D. Clark Turner, E. Bard, C. Jensen, MOXTEK, Inc., Orem, UT</td>
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<td>Q. Qiu, B. Gao, J. Lu, O. Zhou, XINTEK, Inc., Chapel Hill, NC</td>
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<td>2:10</td>
<td>F-41</td>
<td>NEW SEQUENTIAL XRF: PERFORMANCE IMPROVEMENTS THROUGH INNOVATIVE DESIGN</td>
<td>A. Buman, R. Yellepeddi, Thermo Electron Corporation, Dearborn, MI</td>
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<td>2:30</td>
<td>F-55</td>
<td>EQUA ALL—THE NEW STANDARDLESS SOLUTION FOR ENERGY DISPERSIVE X-RAY FLUORESCENCE</td>
<td>K. Behrens, K. Mauser, Bruker AXS GmbH, Karlsruhe, Germany</td>
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<td>2:50</td>
<td>F-45</td>
<td>DIFFRACTIVE KIRKPATRICK-BAEZ OPTIC FOR MICRO X-RAY FLUORESCENCE</td>
<td>B. Verman, B. Kim, D. Wilcox, R. Samokyszyn, L. Jiang, Osmic, Inc., Auburn Hills, MI</td>
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<td>3:10</td>
<td>Break</td>
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<td>3:30</td>
<td>F-46</td>
<td>BENCH TOP X-RAY FLUORESCENCE SPECTROMETERS BASED ON ORTHOGONAL AND TOTAL REFLECTION GEOMETRY FOR EXCITATION</td>
<td>R.E. Ayala Jiménez, Fisichem, Miami, FL</td>
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<td>3:50</td>
<td>D-48</td>
<td>AUTOMATION IN RESEARCH AND PRODUCTION USING X-RAY POWDER DIFFRACTION</td>
<td>J.P. Nicolich, PANalytical, Natick, MA</td>
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<td>4:10</td>
<td>D-104</td>
<td>BRUKER AXS SUPER SPEED SOLUTIONS FOR X-RAY DIFFRACTION APPLICATIONS</td>
<td>U. Preckwinkel, B. He, L. Bruegemann, Bruker AXS, Inc., Madison, WI/ Karlsruhe, Germany</td>
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<td>4:30</td>
<td>D-90</td>
<td>SWAXS SYSTEM-3 : THE NEW GENERATION OF AUTOMATED SMALL- AND WIDE-ANGLE X-RAY SYSTEMS</td>
<td>P. Laggner, R. Koschuch, M. Kriechebaum, Hecus X-ray Systems GmbH, Graz, Austria</td>
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<td>4:50</td>
<td>F-11</td>
<td>THEBEE ELECTRIC FLUXER...WHY YOU SHOULD MAKE IT YOURS!</td>
<td>F. Bouker, Corporation Scientifique Claisse, Quebec, Canada</td>
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# XRD & XRF

**Wednesday p.m.**

**Session C-2 Thin Films**

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

Co-chair: **H. Toraya**, Rigaku Corporation, Tokyo, Japan

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<td>2:00</td>
<td>F-1</td>
<td>WDXRF ANALYSIS OF THIN LAYERS—Invited</td>
<td>M.W. Dirken, PANalytical B.V., Almelo, The Netherlands</td>
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<td>2:30</td>
<td>D-61</td>
<td>GRAZING-INCIDENT X-RAY DIFFRACTION ANALYSES OF NOVEL MAGNETIC THIN FILMS—Invited</td>
<td>K. Inaba, Y. Ito, K. Omote, H. Toraya, Rigaku Corporation, Tokyo, Japan</td>
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<td>3:00</td>
<td>D-12</td>
<td>ULTRA-FAST SIMULTANEOUS FITTING OF SEVERAL BRAGG REFLECTIONS FROM AIA’s/GaAs SUPERLATTICES USING METHOD OF EIGENWAVES</td>
<td>A. Ulyanenkov, R. Eisenhower, I. Feranchuk, H. Guérault, H. Ress, Bruker AXS, Karlsruhe, Germany</td>
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<td>3:20</td>
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<td>Break</td>
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<td>3:50</td>
<td>D-5</td>
<td>THE DIRECT DETERMINATION OF X-RAY DIFFRACTION DATA FROM SPECIFIC DEPTHS</td>
<td>A. Broadhurst, K.D. Rogers, D.W. Lane, T.W. Lowe, Cranfield University, Swindon, UK</td>
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<td>4:10</td>
<td>D-70</td>
<td>“BaF₂ PROCESS”: PHASE EVOLUTION OF Ba₂YCu₅O₆₊ₓ FILMS</td>
<td>W. Wong-Ng, I. Levin, M.D. Vaudin, L.P. Cook, National Institute of Standards &amp; Technology, Gaithersburg, MD</td>
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<td>R. Feenstra, Oak Ridge National Laboratory, Oak Ridge, TN</td>
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<td>4:30</td>
<td>D-89</td>
<td>IN-SITU HTXRD CHARACTERIZATION FOR THIN FILMS</td>
<td>E.A. Payzant, S.A. Speakman, Oak Ridge National Laboratory, Oak Ridge, TN</td>
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XRD

Wednesday p.m.

Session D-1 Small Angle Scattering
Organized by: N.S. Murthy, University of Vermont, Burlington, VT
J.D. Londono, DuPont Company, Wilmington, DE

2:00 D-108 IN SITU STUDIES OF NANO-PARTICLE GROWTH IN FLAMES—Invited
G. Beaucage, N. Agashe, University of Cincinnati, Cincinnati, OH
H.K. Kammler, S.E. Pratsinis, Institute of Process Engineering, ETH Zentrum, Zurich, Switzerland
J. Ilavsky, P. Jemian, UNICAT, Advanced Photon Source, Argonne, IL
T. Narayanan, ID02, European Synchrotron Research Facility, Grenoble, France
D. Londono, DuPont Experimental Station, Wilmington, DE

2:30 D-106 IN-SITU STRUCTURAL STUDIES OF SEMICRYSTALLINE POLYMER BLENDS USING SYNCHROTRON RADIATION—Invited
P. Thiyagarajan, S. Seifert, Argonne National Laboratory, Argonne, IL
M. Kipper, B. Narasimhan, Iowa State University, Ames, IA

3:00 D-91 LOOKING AT SMALL HOLES: CROSS-VALIDATION OF SAXS- AND BET-POROSIMETRY
P. Laggner, Austrian Academy of Sciences, Graz, Austria and Hecus X-ray Systems GmbH, Graz, Austria

3:20 Break

3:40 D-101 FROM LAB TO FAB: THE DEVELOPMENT AND DEPLOYMENT OF NEW METROLOGY TECHNOLOGY FOR THE GLOBAL SEMICONDUCTOR INDUSTRY—Invited
B. Landes, B. Kern, J. Niu, C. Mohler, J. Hahnfeld, D. Yontz, K. Ender, C. Silvis,
R. Strittmatter, L. Moore, T. Stokich, D. King, Dow Chemical Co., Midland, MI
J. Quintana, S. Weigand, Northwestern University, Chicago, IL

4:10 D-56 TIME-RESOLVED SMALL ANGLE SCATTERING STUDIES OF ALIGNMENT OF BLOCK COPOLYMER SOLUTIONS INDUCED BY ELECTRIC FIELDS
V. Urban, Oak Ridge National Laboratories, Oak Ridge, TN
A. Böker, H. Elbs, H. Hänsel, A. Knoll, S. Ludwigs, H. Zettl, V. Abetz, A.H.E. Müller,
G. Krausch, Universität Bayreuth, Bayreuth, Germany

4:30 D-3 SAXSess—AN ANALYTICAL TOOL FOR NANOSTRUCTURED MATERIALS
H. Schnablegger, Anton-Paar GmbH, Graz, Austria
A. Bergmann, O. Glatter, University of Graz, Graz, Austria

4:50 D-15 CRISTALLINE OR LIQUID CRISTALLINE? A XRD STUDY ON OCTASUBSTITUTED DISCOTIC PHTHALOCYANINES
W. Xia, B.A. Minch, M.D. Carducci, N.R. Armstrong, University of Arizona, Tucson, AZ
XRF

Wednesday p.m.  Rainbow

Session F-1 © Quantitative XRF
Organized by: J.V. Gilfrich, Emeritus, SFA, Inc./NRL, Bethesda, MD
Co-Chair: J. Sieber, National Institute of Standards & Technology, Gaithersburg, MD

2:00 F-47  QUANTITATIVE PROCEDURES IN TXRF—Invited
P. Wobrauschek, Atominstitut, Vienna, Austria

2:30 F-25  ADVANCED PULSE PROCESSING AND ANALYTICAL METHODS FOR
QUANTITATIVE ENERGY DISPERSIVE XRF AND MICRO-EDXRF—Invited

3:00 F-19  DEVELOPMENT OF A MONTE CARLO—LIBRARY LEAST-SQUARES (MCLLS)
CODE PACKAGE FOR THE EDXRF INVERSE PROBLEM—Invited
R.P. Gardner, W. Guo, North Carolina State University, Raleigh, NC

3:30 Break

3:50 F-26  MICRO-XRF ANALYSIS OF THIN FILMS AND COATINGS USING
FUNDAMENTAL PARAMETERS

4:10 F-5   THE ROLE OF STANDARDS AUSTRALIA IN ACHIEVING AND MAINTAINING
ACCURACY AND PRECISION IN LITHIUM BORATE FUSION—
XRF SPECTROMETRIC ANALYSIS
J.G.H. Metz, XRF Scientific Pty. Ltd., Victoria, Australia

4:30 F-36  QUANTITATIVE ANALYSIS OF SINGLE PARTICLES BY COMBINATION OF
X-RAY MICROANALYSIS AND MONTE CARLO SIMULATIONS
J. Osán, S. Török, KFKI Atomic Energy Research Institute, Budapest, Hungary
L. Vincze, University of Antwerp, Antwerp, Belgium

4:50 F-18  A MONTE CARLO CODE FOR SIMULATION OF PULSE PILE-UP SPECTRAL
DISTORTION IN PULSE-HEIGHT MEASUREMENT
R.P. Gardner, W. Guo, F. Li, North Carolina State University, Raleigh, NC
**SPECIAL SESSIONS—XRD & XRF**

**Session C-3 Detectors & Sources**

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

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<tr>
<td>9:00</td>
<td>C-7</td>
<td>A NEW ULTRA FAST AND LOW NOISE X-RAY DETECTOR SYSTEM—Invited</td>
<td>K. Omote, A. Tsukiyama, M. Kuraibayashi, T. Saito, Rigaku Corporation, Tokyo, Japan</td>
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<tr>
<td>9:30</td>
<td>C-8</td>
<td>MODELLING THE RESPONSE OF SILICON X-RAY DETECTORS</td>
<td>T. Eggert, Ketek GmbH, München, Germany</td>
</tr>
<tr>
<td>9:50</td>
<td>C-4</td>
<td>IMPROVING ENERGY STABILITY IN THE NIST MICROCALORIMETER X-RAY DETECTOR</td>
<td>T. Jach, J.A. Small, D.E. Newbury, National Institute of Standards &amp; Technology,</td>
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<td></td>
<td>Gaithersburg, MD</td>
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<tr>
<td>10:10</td>
<td></td>
<td>Break</td>
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<td>10:40</td>
<td>F-9</td>
<td>PROGRESS WITH SILICON DRIFT DETECTORS USED FOR HIGH RESOLUTION—HIGH COUNT RATE X-RAY</td>
<td>H. Soltau, P. Lechner, PNSensor GmbH, Muenchen, Germany</td>
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<td>SPECTROSCOPY</td>
<td>G. Lutz, L. Strüder, MPI Halbleiterlabor, Muenchen, Germany</td>
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<td>C. Fiorini, A. Longoni, Politecnico, Milano, Italy</td>
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<tr>
<td>11:00</td>
<td>F-10</td>
<td>LARGE AREA SILICON DRIFT DETECTORS FOR XRF APPLICATIONS</td>
<td>O. Boslau, T. Eggert, P. Goldstraß, J. Kemner, Ketek GmbH, München, Germany</td>
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<td>POWDER DIFRACTOGRAM</td>
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</table>
XRD & XRF

Thursday a.m.

C-4 Synchrotron Applications I
Organized by: C. Lavoie, IBM T.J. Watson Research Center, Yorktown Heights, NY
Co-chair: T. Van Buuren, Lawrence Livermore National Laboratory, Livermore, CA

9:00 D-31 HIGH-RESOLUTION SYNCHROTRON RADIATION XRD AND MICROSTRUCTURE IMAGING IN 6-DIM ORIENTATION-LOCATION SPACE BY THE MOVING AREA DETECTOR METHOD—Invited
L. Wcislak, University of Denver, Denver, CO and National Institute of Standards & Technology, Boulder, CO
H.J. Bunge, Technical University of Clausthal, Germany
H. Klein, University of Gottingen, Germany
U. Garbe, J.R. Schneider, HASYLAB at DESY, Hamburg, Germany

9:30 D-8 MATERIALS SCIENCE APPLICATIONS OF THE THREE DIMENSIONAL X-RAY DIFFRACTION MICROSCOPE
L. Margulies, Risoe National Laboratory, Roskilde, Denmark and European Synchrotron Radiation Facility, Grenoble, France
A. Kvick, European Synchrotron Radiation Facility, Grenoble, France

9:50 D-116 TEXTURE OF NiSi FILMS ON SINGLE CRYSTAL SILICON—Invited
C. Detavernier, IBM T.J. Watson Research Center, Yorktown Heights, NY and Universiteit Gent, Gent, Belgium
C. Lavoie, IBM T.J. Watson Research Center, Yorktown Heights, NY

10:20 Break

10:50 D-63 HIGH ENERGY X-RAY DIFFRACTION INVESTIGATION OF THE FERROELECTRIC BEHAVIOR OF (Pb,La)(Zr,Ti)O₃
R.C. Rogan, E. Üstündag, Iowa State University, Ames, IA
M.R. Daymond, Rutherford-Appleton Laboratory, Didcot, United Kingdom
U. Liebert, Argonne National Laboratory, Argonne, IL

11:10 D-64 IN-SITU STUDY OF OXIDE GROWTH ON A KANTHAL ALLOY
E. Üstündag, Iowa State University, Ames, IA
J.D. Almer, Argonne National Laboratory, Argonne, IL
J. Nychka, D.R. Clarke, University of California, Santa Barbara, CA
XRD

Thursday a.m. Twilight

Session D-2 Stress Analysis
Organized by: C.C. Goldsmith, IBM Microelectronics, Hopewell Junction, NY

8:30 D-105 TRANSIENT STRESS EFFECTS IN THIN FILMS DETERMINED BY X-RAY DIFFRACTION—Invited
C.E. Murray, IBM T.J. Watson Research Center, Yorktown Heights, NY

9:00 D-11 MEASUREMENT AND MODELING OF RESIDUAL STRESSES AT MICROSCOPIC AND MESOSCOPIC LEVELS USING MICRO RAMAN SPECTROSCOPY AND X-RAY DIFFRACTION
B. Benedikt, M. Lewis, P. Rangaswamy, Los Alamos National Laboratory, Los Alamos, NM

9:20 D-22 SIMULTANEOUS EVALUATION OF TOTAL AND THERMAL STRAINS/STRESSES IN THERMALLY CYCLED THIN FILMS
J. Keckes, Erich Schmid Institute for Materials Science, Austria

9:40 D-6 FAST IN-SITU X-RAY DIFFRACTION STRESS ANALYSIS DURING HEAT TREATMENT CYCLES OF STEEL
T.K. Hirsch, A. da Silva Rocha, Stiftung Institut fuer Werkstofftechnik, Bremen, Germany

10:00 D-52 INTERNAL STRAIN PROFILE AROUND THE CRACK TIP AND ITS INFLUENCE ON HYDRIDE FORMATION IN ZIRCALOY-4
E. Garlea, B. Yang, M.M. Morrison, R.A. Buchanan, P.K. Liaw, The University of Tennessee, Knoxville, TN
H. Choo, The University of Tennessee, Knoxville, TN and Oak Ridge National Laboratory, Oak Ridge, TN
D.W. Brown, S. Park, L.L. Daemen, Los Alamos National Laboratory, Los Alamos, NM
C.R. Hubbard, Oak Ridge National Laboratory, Oak Ridge, TN
H.F. Letzring, PPC Industries, Troy, MI

10:20 Break

10:40 D-9 RELAXATION OF RESIDUAL STRESS IN SHOT PEENED Ti-6Al-4V DUE TO FRETTING FATIGUE
S. Martinez, M. Blodgett, Air Force Research Laboratories, WPAFB, OH
S. Sathish, Air Force Research Laboratories, WPAFB, OH and University of Dayton Research Institute, Dayton, OH
S. Mall, Air Force Institute of Technology, WPAFB, OH

11:00 D-53 CHANGES IN ELASTIC STRAIN PROFILES AROUND A CRACK TIP DURING TENSILE LOADING AND UNLOADING CYCLES
Y. Sun, P.K. Liaw, Y.L. Lu, B. Yang, University of Tennessee, Knoxville, TN
H. Choo, University of Tennessee, Knoxville, TN and Oak Ridge National Laboratory, Oak Ridge, TN
D. W. Brown, Los Alamos National Laboratory, Los Alamos, NM

11:20 D-84 IMPACT OF DIFFERENT STRENGTHENING MECHANISMS ON INTERGRANULAR STRAINS IN DEFORMED ALUMINUM ALLOYS
C.R. Hubbard, J. Pang, Oak Ridge National Laboratory, Oak Ridge, TN
T.A. Saleh, J.W. Jeon, P.K. Liaw, University of Tennessee, Knoxville, TN
H. Choo, Oak Ridge National Laboratory, Oak Ridge, TN and University of Tennessee, Knoxville, TN
D.W. Brown, M.A.M. Bourke, LANSCE, Los Alamos National Laboratory, Los Alamos, NM
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<td>11:40</td>
<td>D-57</td>
<td>LATTICE STRAIN DEVELOPMENT AND STRAIN-INDUCED PHASE TRANSFORMATION DURING FATIGUE OF A COBALT-BASED SUPERALLOY</td>
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<td>M.L. Benson, T.A. Saleh, P.K. Liaw, H. Choo, R.A. Buchanan, The University of Tennessee, Knoxville, TN</td>
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<td>X.-L. Wang, A.D. Stoica, Oak Ridge National Laboratory, Oak Ridge, TN</td>
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<td>M.R. Daymond, Rutherford Appleton Laboratory, OX, UK</td>
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<td>D.W. Brown, Los Alamos National Laboratory, Los Alamos, NM</td>
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<td>D.L. Klarstrom, Haynes International, Inc., Kokomo, IN</td>
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<td>12:00</td>
<td>D-37</td>
<td>RESIDUAL MICROSTRESS DISTRIBUTION IN TEXTURED METAL MATERIALS: METHOD OF STUDY AND REVEALED PRINCIPLES</td>
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<td>Yu. Perlovich, M. Isaenkova, V. Fesenko, Moscow Engineering Physics Institute [State University], Moscow, Russia</td>
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**XRF**

Thursday a.m.  
**Session F-2 | Problem Solving/Industrial Applications of XRF**  
Organized by: **J.A. Anzelmio**, Anzelmo & Associates, Madison, WI

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<th>Speaker(s)</th>
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<tr>
<td>9:00</td>
<td>F-58</td>
<td>XRF APPLICATIONS IN THE SILICA INDUSTRY—Invited</td>
<td>M.L. Paige</td>
<td>U.S. Silica Company, Berkeley Springs, WV</td>
</tr>
<tr>
<td>9:30</td>
<td>F-57</td>
<td>APPLICATIONS OF SAMPLE/SPECIMEN PREPARATION FOR XRF ANALYSIS IN THE CEMENT AND CONCRETE INDUSTRIES—Invited</td>
<td>D. Broton</td>
<td>Construction Technology Laboratories, Skokie, IL</td>
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<tr>
<td>10:00</td>
<td>F-4</td>
<td>MICRO WDXRF AND ITS INDUSTRIAL APPLICATIONS</td>
<td>N. Gao, Z. Chen, D.M. Gibson</td>
<td>X-Ray Optical Systems, Inc., Albany, NY</td>
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<td>10:20</td>
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<td>Break</td>
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<td>10:50</td>
<td>F-20</td>
<td>ANALYSIS OF TOXIC METALS IN PLASTICS FOR COMPLIANCE WITH ENVIRONMENTAL REGULATIONS</td>
<td>S. Piorck</td>
<td>Niton LLC, Billerica, MA</td>
</tr>
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<td>11:10</td>
<td>F-14</td>
<td>PROCEDURE TO CONSIDER FOR FUSING COPPER/IRON SULFIDE CONCENTRATES</td>
<td>J.P. Gagnon</td>
<td>Corporation Scientifique Claisse, Ste-Foy, Quebec, Canada</td>
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<tr>
<td>11:30</td>
<td>F-23</td>
<td>XRF ANALYSIS OF HARMFUL METALS COLLECTED ONTO FILTERS AS THIN LAYERS FROM WORKPLACE AIR: INTER-LABORATORY EXERCISE</td>
<td>R. Foster</td>
<td>Health and Safety Laboratory, Sheffield, United Kingdom</td>
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**XRD & XRF**

Thursday p.m.  

*Session C-5 Synchrotron Applications II*

Organized by: C. Lavoie, IBM T.J. Watson Research Center, Yorktown Heights, NY  
Co-chair: T. Van Buuren, Lawrence Livermore National Laboratory, Livermore, CA

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<td>2:00</td>
<td>C-6</td>
<td>PROBING THE PHYSICAL AND ELECTRONIC PROPERTIES OF NANOMATERIALS—Invited</td>
<td>T. van Buuren, Lawrence Livermore National Laboratory, Livermore, CA</td>
</tr>
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</table>
| 2:30  | F-35         | COMPARISON OF COMPUTED ABSOLUTE FLUORESCENCE PHOTON COUNTS WITH DATA FROM FULLY CALIBRATED BEAMLINES AND DETECTORS AT PTB/BESSY-II | M. Mantler, Vienna University of Technology, Vienna, Austria  
B. Beckhoff, M. Kolbe, G. Ulm, Physikalisch Technische Bundesanstalt, Berlin, Germany |
| 2:50  | D-30         | IN-SITU HIGH TEMPERATURE (UP TO 1650°C), IN AIR, X-RAY DIFFRACTION (REFLECTION GEOMETRY) USING A QUADRUPOLE LAMP FURNACE | P. Sarin, K. Jurkschat, W.M. Kriven, University of Illinois at Urbana-Champaign, Urbana, IL  
P. Zschack, University of Illinois at Urbana-Champaign, Urbana, IL and Argonne National Laboratory, Argonne, IL |
| 3:10  | Break        |                                                                                           |                                                                                      |
| 3:40  | F-7          | ELEMENT-IDENTIFIED THREE-DIMENSIONAL ATOMIC IMAGING BY COMPLEX X-RAY HOLOGRAPHY           | Y. Takahashi, K. Hayashi, E. Matsubara, Tohoku University, Miyagi, Sendai, Japan       |
| 4:00  | F-56         | DETAILED CORRECTION PROCEDURE FOR X-RAY SPECTROSCOPIC DATA COLLECTED AT A SYNCHROTRON RADIATION FACILITY: SIMULATIONS AND EXPERIMENT | J.M. Ablett, C.-C. Kao, NSLS, Brookhaven National Laboratory, Upton, NY  
J.C. Woick, APS, Argonne National Laboratory, Argonne, IL |
| 4:20  | D-23         | IN-SITU SYNCHROTRON WAXS ON WOOD FOILS AND ON INDIVIDUAL WOOD CELLS COMBINED WITH MICROSENSILE TESTS | J. Keckes, Erich Schmid Institute for Materials Science, Austria  
I. Burgert, P. Fratzl, Max-Planck-Institute of Colloids and Interfaces, Potsdam, Germany  
M. Müller, K. Kölln, University Kiel, Germany  
S.V. Roth, European Synchrotron Radiation Facility, Grenoble, France  
S.E. Stanzl-Tschegg, University of Agricultural Sciences, Vienna, Austria |
XRD & XRF

Thursday p.m. 

Session C-6 X-ray Optics
Organized by: S.T. MISTURE, NYS College of Ceramics at Alfred University, Alfred, NY

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<tr>
<td>2:00</td>
<td>F-31 POLYCAPILLARY OPTICS IN MICRO X-RAY FLUORESCENCE—Invited</td>
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<td>G.J. Havrilla, Los Alamos National Laboratory, Los Alamos, NM</td>
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<td>2:30</td>
<td>D-112 QUANTITATIVE EVALUATION OF GRADED PARABOLIC MULTILAYER OPTICS—</td>
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<tr>
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<td>Invited</td>
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<td>J.P. Cline, D. Windover, A. Henins, National Institute of Standards &amp; Technology, Gaithersburg, MD</td>
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<td>3:00</td>
<td>C-3 FOCUSsing FOR MORE FLUX OR HOW TO SHAPE X-RAYS</td>
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<td>A. Dariel, V. Roger, R. Siebrecht, D. Cenda, C. Montcalm, P. Høghøj, XENOCS SA, Sassenage, France</td>
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<td>3:20</td>
<td>Break</td>
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<td>3:50</td>
<td>D-19 HIGH ENERGY EDGE-ENHANCED IMAGING WITH BROADBAND X-RAYS</td>
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<td>K. Fezzaa, W.-K. Lee, J. Wang, APS, Argonne National Laboratory, Argonne, IL</td>
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<td>4:10</td>
<td>D-17 RECENT DEVELOPMENTS OF MULTILAYER OPTICS FOR X-RAY DIFFRACTOMETRY</td>
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<td>A. Bauer, C. Michaelsen, A. Oehr, C. Hoffmann, J. Wiesmann, Incoatec GmbH, Geesthacht, Germany</td>
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<td>A. Storm, L. Seijbel, Bruker Nonius B.V., Delft, The Netherlands</td>
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XRD

Session D-3  Industrial Applications of XRD
Organized by: R.L. Snyder, Georgia Institute of Technology, Atlanta, GA
C.R. Hubbard, Oak Ridge National Laboratory, Oak Ridge, TN

2:00 D-13 XRD INVESTIGATIONS IN ANHYDROUS AND HYDROUS CEMENTITIOUS SYSTEMS—Invited
H. Pöllmann, University of Halle, Halle, Germany

2:30 D-99 CHARACTERIZATION OF STRUCTURED FLUIDS DURING FLOW BY SMALL ANGLE NEUTRON SCATTERING—Invited
A.I. Nakatani, Rohm and Haas Company, Spring House, PA

3:00 D-100 IN-SITU STRUCTURE DEVELOPMENT DURING THE MELT SPINNING OF NYLON 66—Invited
J.D. Londono, H. Chang, R.V. Davidson, J. Potter, DuPont Company, Wilmington, DE

3:30 Break

3:50 D-21 BAYESIAN CHARACTERISATION OF NANOCRYSTALLITES FROM LINE PROFILE DATA
N. Armstrong, W. Kalceff, A.R. Dowd, University of Technology Sydney, NSW, Australia
J.P. Cline, National Institute of Standards & Technology, Gaithersburg, MD

4:10 D-75 QUANTITATIVE ANALYSIS OF CALCIUM OXIDE DESICCANT CONVERSION TO CALCIUM HYDROXIDE USING X-RAY DIFFRACTION
T.N. Blanton, C.L. Barnes, Eastman Kodak Company, Rochester, NY

4:30 D-110 EFFECT OF CRYSTAL SIZE ON QUANTITATIVE ESTIMATION OF SILICA POLYMORPHS IN SILICA BRICKS BY X-RAY DIFFRACTION
P. Sahu, B.K. Panda, J.D. Panda, Dalmia Institute of Scientific and Industrial Research, Orissa, India

4:50 D-58 DEVELOPMENT OF XRD IN EL SALVADOR
E. de Henriquez, LaGeo S.A. de C.V., El Salvador, Central America

5:10 D-41 TWO-DIMENSIONAL MAPPING OF RESIDUAL STRESSES IN 6061-T6 ALUMINUM FRICTION STIR WELDS
W. Woo, P. K. Liaw, University of Tennessee, Knoxville, TN
H. Choo, University of Tennessee, Knoxville, TN and Oak Ridge National Laboratory, Oak Ridge, TN
D. W. Brown, Los Alamos National Laboratory, Los Alamos, NM
Z. Feng, S.A. David, C.R. Hubbard, Oak Ridge National Laboratory, Oak Ridge, TN
**XRF**

Thursday p.m.  

Session F-3 y Trace Analysis  
Organized by: M.A. Zarrz, IBM, Hopewell Junction, NY

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<td>2:00</td>
<td>F-27</td>
<td>TXRF—VERSATILE APPLICATIONS IN DEPTH PROFILING, SPECIATION BY XANES AND ULTRA TRACE ELEMENT ANALYSIS INCLUDING LOW Z ELEMENTS—Invited</td>
<td>C. Streli, Atominstitut, Vienna University of Technology, Wien, Austria</td>
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<tr>
<td>2:30</td>
<td>F-28</td>
<td>TRACE ELEMENT ANALYSIS USING A BENCHTOP TXRF-SPECTROMETER—Invited</td>
<td>H. Stosnach, Röntec GmbH, Berlin, Germany</td>
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<td>3:00</td>
<td>F-15</td>
<td>CHARACTERIZING HAFNIUM SILICATE GATE DIELECTRICS WITH A TOTAL REFLECTION X-RAY FLUORESCENCE SPECTROMETER</td>
<td>C. Sparks, P. Lysaght, T. Rhoad, International SEMATECH, Austin, TX</td>
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<td>3:20</td>
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<td>Break</td>
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<td>3:50</td>
<td>F-12</td>
<td>PPB ANALYSIS BY XRF: A NEW MICRO-DROPLET METHOD FOR ENVIRONMENTAL LIQUID SAMPLE</td>
<td>T. Moriyama, Y. Yamada, H. Kohno, Rigaku Industrial Corporation, Takatsuki, Osaka, Japan</td>
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<td>H. Inoue, J.E. Martin, Rigaku/MSC Inc., The Woodlands, TX</td>
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<td>4:10</td>
<td>F-32</td>
<td>MICRO X-RAY FLUORESCENCE AS AN ANALYTICAL TOOL IN CASHMERE HAIR CHARACTERIZATION</td>
<td>S. Wiltshire, G.J. Havrilla, T. Miller, Los Alamos National Laboratory, Los Alamos, NM</td>
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<td>D. Exline, R.J. Lee Group, Inc., Monroeville, PA</td>
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### XRD & XRF

**C-7 Microbeam Analysis**  
Organized by: **G.J. Havrilla**, Los Alamos National Laboratory, Los Alamos, NM  
**T. Miller**, X-ray Optical Systems, Inc., East Greenbush, NY

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| 8:30 | F-38    | COMBINATION OF SCANNING PROBE MICROSCOPE AND X-RAY ANALYSIS—Invited   | K. Tsuji, T. Emoto, Y. Matsuoka, Osaka City University, Osaka, Japan  
Y. Miyatake, T. Nagamura, Unisaku Co., Hirakata, Japan  
X. Ding, Beijing Normal University, Beijing, China |
| 9:00 | D-109   | SAMPLING VOLUME CONCERNS IN MICRO X-RAY DIFFRACTION—Invited           | I.C. Noyan, IBM T.J. Watson Research Center, Yorktown Heights, NY                      |
| 9:30 | D-32    | X-RAY MICRODIFFRACTION STUDIES OF CORROSION SCALES IN OLD IRRON/STEEL DRINKING WATER DISTRIBUTION PIPES | P. Sarin, V.L. Snoeyink, W.M. Kriven, University of Illinois at Urbana-Champaign, Urbana, IL  
D. Hay, CSIRO Manufacturing and Infrastructure Technology, Clayton, Victoria, Australia |
| 9:50 | D-62    | X-RAY MICRODIFFRACTION STUDY OF INDENTATION INDUCED FRACTURE IN SINGLE CRYSTAL BaTiO₃ | R.C. Rogan, E. Üstündag, M.A. Brown, Iowa State University, Ames, IA  
N. Tamura, Lawrence Berkeley National Laboratory, Berkeley, CA |
| 10:10|        | Break                                                               |                                                                                       |
| 10:30| F-2     | MICRO X-RAY FLUORESCENCE IMAGING OF PHARMACEUTICAL TABLET FORMULATIONS | T. C. Miller, X-ray Optical Systems, Inc., East Greenbush, NY  
G.J. Havrilla, Los Alamos National Laboratory, Los Alamos, NM |
| 10:50| F-6     | A NOVEL APPLICATION OF PULSED X-RAY IN LASER MATTER INTERACTION      | F. A. Selim, D.P. Wells, J.F. Harmon, Idaho State University, Pocatello, ID          |
| 11:10| F-17    | DETECTION OF LATENT HUMAN FINGERPRINTS BY MICRO-X-RAY FLUORESCENCE   | C.G. Worley, S.S. Wiltshire, T.C. Miller, G.J. Havrilla, V. Majidi, Los Alamos National Laboratory, Los Alamos, NM |
| 11:30| F-30    | CONFOCAL X-RAY FLUORESCENCE MICROSCOPE                              | G. J. Havrilla, Los Alamos National Laboratory, Los Alamos, NM  
N. Gao, X-ray Optical Systems, Inc., East Greenbush, NY |
| 11:50| F-50    | ELEMENTAL DISTRIBUTION IN VARIOUS AREAS OF HUMAN ARTICULAR BONES BY SR µ-XRF | N. Zoeger, P. Wobrauschek, C. Streli, C. Jokubonis, Atominstitut, Vienna University of Technology, Vienna, Austria  
G. Pepponi, ITC-irst, Trento, Italy  
P. Roschger, Ludwig Boltzmann-Institut für Osteologie, Vienna, Austria  
G. Falkenberg, HASYLAB at DESY, Hamburg, Germany  
W. Osterode, Universitätsklinik für Innere Medizin IV, Vienna, Austria |
## XRD

**Session D-4 Parallel Beam Diffraction**

Organized by: **R.L. Snyder**, Georgia Institute of Technology, Atlanta, GA  
**S.T. Misture**, NYS College of Ceramics at Alfred University, Alfred, NY

<table>
<thead>
<tr>
<th>Time</th>
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<tbody>
<tr>
<td>8:30</td>
<td>D-117 PARALLEL BEAM XRD: HIGH ACCURACY DATA FROM POWDERS AND POLYCRYSTALLINE THIN FILMS—Invited</td>
</tr>
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<td>D.K. Bowen, Bede Scientific, Inc., Englewood, CO</td>
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<tr>
<td>9:00</td>
<td>D-65 A REVIEW OF COMPACT, LOW-POWER, ON-LINE, DIFFRACTION-BASED ANALYZERS—Invited</td>
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<tr>
<td></td>
<td>H. Huang, W.M. Gibson, X-ray Optical Systems, Inc., East Greenbush, NY</td>
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<tr>
<td>9:30</td>
<td>D-34 FUNDAMENTAL PARAMETERS FITTING OF XRPD DATA MEASURED USING MULTILAYER OPTICS</td>
</tr>
<tr>
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<td>S.T. Misture, M.D. Dolan, NYS College of Ceramics at Alfred University, Alfred, NY</td>
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<tr>
<td>9:50</td>
<td>D-50 PARALLEL BEAM GEOMETRY AFTER THE HYPE</td>
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<td>M. Fransen, PANalytical, Almelo, The Netherlands</td>
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<td>10:10</td>
<td>Break</td>
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<tr>
<td>10:30</td>
<td>D-77 TOWARDS FAST RECIPROCAL SPACE MAPPING</td>
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<td>J.F. Woitok, A. Kharchenko, PANalytical B.V., Almelo, The Netherlands</td>
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<tr>
<td>10:50</td>
<td>D-98 STRATEGIES FOR PARALLEL BEAM DIFFRACTION ANALYSIS OF MESOPOROUS THIN FILMS</td>
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<td>K. Macchiarola, C. Reiss, B. Kinneging, PANalytical, Natick, MA</td>
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## Session D-5 Rietveld Applications
Organized by: J.A. Kaduk, BP Chemicals, Naperville, IL

<table>
<thead>
<tr>
<th>Time</th>
<th>Paper</th>
<th>Title</th>
<th>Authors</th>
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<tr>
<td>8:30</td>
<td>D-103</td>
<td>ACCURATE DETERMINATION OF ORGANIC CRYSTAL STRUCTURES FROM POWDER DIFFRACTION DATA—Invited</td>
<td>W.I.F. David, Rutherford Appleton Laboratory, Oxfordshire, United Kingdom</td>
</tr>
<tr>
<td>9:00</td>
<td>D-111</td>
<td>CRYSTAL CHEMISTRY AND ENERGETICS OF NEW NaNbO₃—BASED PEROVSKITES—Invited</td>
<td>H. Xu, A. Navrotsky, University of California at Davis, Davis, CA and Y. Su, M.L. Balmer, Pacific Northwest National Laboratory, Richland, WA</td>
</tr>
<tr>
<td>9:30</td>
<td>D-71</td>
<td>BaF₂ PROCESS OF LONG-LENGTH CONDUCTORS: HIGH-TEMPERATURE NEUTRON AND X-RAY STUDY OF YOF</td>
<td>W. Wong-Ng, I. Levin, Q. Huang, L.P. Cook, National Institute of Standards &amp; Technology, Gaithersburg, MD</td>
</tr>
<tr>
<td>9:50</td>
<td>D-4</td>
<td>CRYSTAL STRUCTURE OF GUAIFENESIN, 3-(2-METHOXYPHENOXY)-1,2-PROPANEDIOL</td>
<td>J.A. Kaduk, BP Chemicals, Naperville, IL</td>
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<td>10:10</td>
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<td>Break</td>
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</tr>
<tr>
<td>10:50</td>
<td>D-113</td>
<td>PHASE TRANSFORMATION TEXTURES IN Ti-6AI-4V ALLOY</td>
<td>S.C. Vogel, D.J. Williams, Los Alamos National Laboratory, Los Alamos, NM and D. Bhattacharyya, G.B. Viswanathan, H.L. Fraser, Ohio State University, Columbus, OH</td>
</tr>
<tr>
<td>11:10</td>
<td>D-83</td>
<td>POWDER DIFFRACTION ANALYSIS OF HYDRAULIC CEMENTS: ASTM Rietveld Round Robin for Precision and Bias</td>
<td>P. Stutzman, National Institute of Standards and Technology, Gaithersburg, MD</td>
</tr>
<tr>
<td>11:30</td>
<td>D-59</td>
<td>INVESTIGATION OF REACTION KINETICS IN CERAMIC SYSTEMS USING HIGH-TEMPERATURE X-RAY DIFFRACTION</td>
<td>M.D. Dolan, S.T. Misture, NYS College of Ceramics at Alfred University, Alfred, NY</td>
</tr>
</tbody>
</table>
XRD

Session D-6 Polymers
Organized by: N.S. Murthy, University of Vermont, Burlington, VT
K.H. Gardner, DuPont Company, Wilmington, DE

8:00 D-118 STRUCTURE OF POLYMERS USING NEUTRON AND X-RAY FIBER DIFFRACTION—Invited
T. Forsyth, Institut Laue Langevin, Grenoble, France, and Keele University, Staffordshire, UK

8:30 D-76 SIMULTANEOUS SAXS/WAXD STUDY OF IN-SITU POLYMER PROCESSING—Invited
B.S. Hsiao, State University of New York, Stony Brook, NY

9:00 D-107 ORIENTED ANTHRACENE AND PENTACENE THIN FILMS—Invited
R.L. Headrick, H. Zhou, University of Vermont, Burlington, VT
R. Ruiz, A.C. Mayer, G.G. Malliaras, Cornell University, Ithaca, NY
A. Kazimirov, Cornell High Energy Synchrotron Source, Ithaca, NY

9:30 D-97 MEASUREMENT OF LARGE CRYSTALLITE SIZES IN POLY(OXYMETHYLENE)
R. Barton, Jr., DuPont Experimental Station, Wilmington, DE
J.R. Lawson, DuPont Engineering Polymers, Parkersburg, WV

9:50 Break

10:10 D-119 STRUCTURE DETERMINATION OF POLYMER FIBER USING DIRECT METHOD TECHNIQUES—Invited
K.H. Gardner, DuPont Company, Wilmington, DE

10:40 D-74 X-RAY SCATTERING AND DSC STUDIES OF PRE-MELTING CRYSTALLIZATION BEHAVIOR IN NYLON 6—Invited
S.T. Correale, Honeywell International, Inc., Petersburg, VA
N.S. Murthy, Honeywell Laboratories, Morristown, NJ

11:10 D-47 TEMPERATURE EXPERIMENTS FOR IMPROVING ACCURACY IN THE CALCULATION OF THE DEGREE OF CRYSTALLINITY OF POLYAMIDE-11
P. Ricou, E. Pinel, N. Juhasz, ATOFINA Chemicals, Inc., King of Prussia, PA

11:30 D-40 STRESSES IN SHAPE MEMORY POLYMER MATRIX COMPOSITES FOR BIOMEDICAL APPLICATIONS
D. Balzar, University of Denver, Denver, CO and National Institute of Standards & Technology, Boulder, CO
K. Gall, M.L. Dunn, Y. Liu, University of Colorado, Boulder, CO

11:50 D-1 3D STRUCTURE OF DENDRITIC AND HYPER-BRANCHED MACROMOLECULES BY X-RAY DIFFRACTION
V. Petkov, Central Michigan University, Mt. Pleasant, MI
**Summer Activities**

Information and reservations for these and many other local activities are available through the Sheraton Steamboat Concierge Desk. Our knowledgeable staff is here to help you make great memories!

**WORLD CLASS FLY FISHING:** Fly or cast fishing is a must in Steamboat. Fish at Steamboat Lake, Stagecoach Reservoir or on the Elk and Yampa rivers.

**HIKING:** Steamboat offers many attractions for all levels of hiking: Fish Creek Falls, Mount Zirkel Wilderness and many State Parks in the area.

**DINNER WAGON RIDES:** Round up your group for an old-fashioned wagon ride and dinner in the midst of a mountain paradise. You'll be treated to a ride in a horse-drawn wagon, dinner and dessert. What a great way to end the day!

**HOT AIR BALLOON RIDES:** Daily, weather permitting, 1/2 hour & one hour tours, complimentary transportation.

**PRO RODEO SERIES:** During the summer the Pro Rodeo series comes to Steamboat every Friday and Saturday night at 7:30pm, June through August at the Howelsen Hill Rodeo Grounds.

**ATV TOURS:** Take an ATV tour of Routt National Forest, with trails and terrain suitable for dirt bikes and ATVs.

**WHITESTREAM RAFTING, TUBING, KAYAKING:** Many options, from tranquil to exhilarating, 5 to 90 minutes away.

**ROCK CLIMBING:** Daily, half & full day tours, 3 day and 6 day rock climbing camps, climbing instruction and guided climbs.

**MOUNTAIN BIKING:** The terrain surrounding Steamboat offers great riding for both mountain and road bikers. From the bike and pedestrian trail system to the world-class mountain trails, there is something for every type of cyclist.

**SHERATON STEAMBOAT RESORT GOLF RESORT:** Robert Trent Jones, II championship course owned by the Sheraton and operated by Troon Golf. Additionally, Steamboat offers the Haymaker, Lake Catamount and Steamboat Golf Club courses.

**SWIMMING/WATERSLIDE:** At the end of an active day, a relaxing soak in a natural hot springs mineral pool is just what those sore muscles need. For those in the group who still crave excitement, the 350 foot hydrotube will start the adrenaline!

**GONDOLA SQUARE:** Just steps from our door you can... play Frisbee golf, bounce on the bungee tramp, scale the climbing wall, hike or bike Mt. Werner and ride the Silver Bullet Gondola.

**HORSEBACK RIDING:** Be a part of Steamboat's western heritage! Enjoy the fantastic scenery while you ride trails set in our surrounding wilderness areas and national forests.

**HOWLER ALPINE SLIDE:** Join the fun on historic Howelsen Hill on a two-track, 2400 foot slide of summertime fun!

Sheraton Steamboat
RESORT & CONFERENCE CENTER

Sheraton Steamboat Resort – 2200 Village Inn Court – P.O. Box 14808 – Steamboat Springs, CO 80477
Main Phone: (970) 879-2220 Concierge Extension: 1005 Fax: (970) 879-7666 Sales Phone: (800) 819-2884 Fax: (970) 879-4988
SCENIC DRIVE – Steamboat Springs is located just 169 miles from Denver International Airport (DIA), a pleasant 3 hour drive. From Denver, travel west on I-70 through the Eisenhower Tunnel to the Silverthorne/Dillon exit. From Silverthorne/Dillon, drive north on Colorado Highway 9 for 36 miles to the town of Kremmling. In Kremmling, turn west onto US Highway 40. Once on US Highway 40, it is just 53 miles to Steamboat Springs. En route, you will pass through the Rockies’ high plains and grazing lands before you begin a gradual ascent over the famed Rabbit Ears Pass. Be sure to look for the “ears” rock formation on your right. After entering Steamboat, take the Mt. Werner exit to the ski area base and the Sheraton Steamboat Resort.
## Denver X-ray Conference Program-at-a-Glance
### 2–6 August 2004

<table>
<thead>
<tr>
<th>Sun. eve.</th>
<th>6:00 – 8:00 Welcoming Reception sponsored by SPEX CertiPrep, Corporation Scientifique Claiisse &amp; Wiley</th>
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</thead>
<tbody>
<tr>
<td><strong>Day &amp; Time</strong></td>
<td><strong>XRD &amp; XRF</strong></td>
</tr>
<tr>
<td><strong>Mon. am:</strong> Functions, 9:00 – 12:00</td>
<td>W1 How to do Synchrotron Experiments (Noyan/Misture/Kaduk) (Rainbow)</td>
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<tr>
<td><strong>Mon. pm:</strong> Workshops, 2:00 – 5:00</td>
<td>W5 X-ray Physics (Elam) (Rainbow)</td>
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<tr>
<td><strong>Mon. eve.</strong></td>
<td>6:00 – 8:00 Evening Reception sponsors to be announced.</td>
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<tr>
<td><strong>Tue. am:</strong> Workshops, 9:00 – 12:00</td>
<td>W9 Microbeam X-ray Stress Analysis (Noyan) (Rainbow)</td>
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<tr>
<td><strong>Tue. pm:</strong> Workshops, 2:00 – 5:00</td>
<td>W13 Principles &amp; Use of MicroXRD &amp; XRF (Blanton) (Rainbow)</td>
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<td><strong>Tue. eve.</strong></td>
<td>6:00 – 8:00 Evening Reception sponsored by MDI &amp; Rigaku</td>
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<td><strong>Wed. am:</strong> 8:30 Plenary Session, Red Hot X-rays (Prewitt/Snyder) Steamboat Grand Hotel</td>
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<tr>
<td><strong>Wed. pm:</strong> Sessions*</td>
<td>C1 New Developments in XRD &amp; XRF Instr. (Anzelmo) (Storm Peak)</td>
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<td><strong>Wed. eve:</strong> 6:00 – 8:00 Evening Reception sponsored by Bruker AXS, Inc.</td>
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<td><strong>Fri. am:</strong> Sessions*</td>
<td>C3 Detectors &amp; Sources (Huang) (Skyline)</td>
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<td>C4 Synchrotron Applications I (Lavoie) (Rainbow)</td>
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<td><strong>Fri. pm:</strong> Sessions*</td>
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<td>C5 Synchrotron Applications II (Lavoie) (Rainbow)</td>
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<td>C6 X-ray Optics (Misture) (Storm Peak)</td>
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<td><strong>Thurs. am:</strong> Sessions*</td>
<td>C7 Microbeam Analysis (Havrilla/Miller) (Rainbow)</td>
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<tr>
<td><strong>Thurs. pm:</strong> Sessions*</td>
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*Session times vary; please consult the Program for exact presentation times.
RESERVATION REQUEST FOR AIR TRAVEL
DENVER X-RAY CONFERENCE
SPONSORED BY
INTERNATIONAL CENTRE FOR DIFFRACTION DATA

STEAMBOAT SPRINGS, COLORADO
AUGUST 2 TO 6, 2004

TRAVELERS NAME: ________________________________

ADDRESS: ______________________________________

PHONE: ___________________ FAX: ____________________

DEPARTURE CITY: ___________________ DEPARTURE DATE: ____________

RETURN CITY: ___________________ RETURN DATE: ________________

DEPARTURE TIME: ________________ RETURN TIME: _______________

AIRLINE PREFERENCE/FREQUENT FLYER NUMBER: ____________________

FORM OF PAYMENT: ________________________________________

SEAT REQUEST PREFERENCE: ________________________________

OTHER: ____________________________________________________

Kitty Ward Travel, Inc. has negotiated special meeting fares with United Airlines. Please book your reservations as soon as possible since space is limited.

United Airlines Reference # 524AE
mward@kittywardtravel.com

Please fax your request form to 610-543-0786 or call 610-543-0680 or 800-752-3718 Out of State.
2004 Denver X-ray Conference Registration Form
Sheraton Steamboat Resort, Steamboat Springs, Colorado, U.S.A.
2–6 August 2004

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 5 July 2004.

Registration Fees:

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<tr>
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<th>after July 5</th>
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<tr>
<td>Full week: exhibits, workshops, sessions†</td>
<td>$375</td>
<td>$450</td>
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<tr>
<td>Monday &amp; Tuesday: exhibits, workshops‡</td>
<td>$325</td>
<td>$400</td>
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<tr>
<td>Wed., Thurs. &amp; Friday: exhibits, sessions‡</td>
<td>$325</td>
<td>$400</td>
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<tr>
<td>Session organizers, invited speakers &amp; workshop instructors†</td>
<td>$100</td>
<td>$100</td>
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<tr>
<td>(Circle one) Students, unemployed, and persons 65 and older‡: full week—exhibits, workshops, sessions</td>
<td>$75</td>
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†Includes a copy of Volume 48 of Advances in X-ray Analysis on CD-ROM
‡Students, unemployed and over 65 must have their status confirmed by phone, fax, e-mail 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 on CD-ROM

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Power Diffraction‡

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Student pricing

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‡See further information regarding Power Diffraction on page 2 of this program.

Please check this box if you do not want your name included on the attendee list.

Are you primarily interested in XRD or XRF topics?

☐ XRD  ☐ XRF  ☐ Equally interested in both

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

Name ____________________________________________
Organization _____________________________________
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Payment:

Total Amount Due: __________________

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◆ E-mail dxc@icdd.com ◆ Phone 610.325.9814 ◆ Fax 610.325.9823

Return by 5 July 2004

On-line registration also available at: www.dxicdd.com