

INTERNATIONAL CENTRE FOR DIFFRACTION DATA

# Denver X-ray Conference



**65<sup>th</sup> Annual**  
**Conference on Applications**  
**of X-ray Analysis**

• • •

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

**1-5 August 2016**

The Westin O'Hare Hotel  
Rosemont, Illinois, USA

## DXC 2016 Program

The information contained in this PDF is current as of March 2016. Updates to the technical Program can be viewed on the Program page of our website:

[WWW.DXCICDD.COM](http://WWW.DXCICDD.COM)

Please be sure to monitor our website for the latest conference information.

Abstracts for Poster presentation will continue to be accepted up until July 20<sup>th</sup>. Please visit the Abstract page of our website to submit your abstract.

Sponsored by



# DENVER X-RAY CONFERENCE ORGANIZING COMMITTEE

**W. Tim Elam**, Chair, University of Washington APL, Seattle, WA, [wtelam@apl.washington.edu](mailto:wtelam@apl.washington.edu)

**Tom Blanton**, Co-chair, ICDD, Newtown Square, PA, [tblanton@icdd.com](mailto:tblanton@icdd.com)

**John Anzelmo**, Anzelmo & Associates, Inc., Madison, WI, [jaanzelmo@aol.com](mailto:jaanzelmo@aol.com)

**Lora Brehm**, Dow Chemical Company, Midland, MI, [lbrehm@dow.com](mailto:lbrehm@dow.com)

**Don Broton**, Construction Technology Labs, Skokie, IL, [dbroton@ctlgroup.com](mailto:dbroton@ctlgroup.com)

**Tim Fawcett**, ICDD, Newtown Square, PA, [fawcett@icdd.com](mailto:fawcett@icdd.com)

**James A. Kaduk**, Poly Crystallography Inc. & Illinois Institute of Technology, Naperville, IL, [kaduk@polycrystallography.com](mailto:kaduk@polycrystallography.com)

**Terry Maguire**, ICDD, Newtown Square, PA, [maguire@icdd.com](mailto:maguire@icdd.com)

**Scott Misture**, NYS College of Ceramics at Alfred University, Alfred, NY, [misture@alfred.edu](mailto:misture@alfred.edu)

**Conal Murray**, IBM T.J. Watson Research Center, Yorktown Heights, NY, [conal@us.ibm.com](mailto:conal@us.ibm.com)

**Cev Noyan**, Columbia University, New York, NY, [icn2@columbia.edu](mailto:icn2@columbia.edu)

**Brian Toby**, Argonne National Laboratory, Advanced Photon Source, Argonne, IL, [brian.toby@anl.gov](mailto:brian.toby@anl.gov)

**Rene van Grieken**, University of Antwerp, Antwerp, Belgium, [rene.vangrieken@ua.ac.be](mailto:rene.vangrieken@ua.ac.be)

**Mary Ann Zaitz**, IBM, Hopewell Junction, NY, [zaitz@us.ibm.com](mailto:zaitz@us.ibm.com)

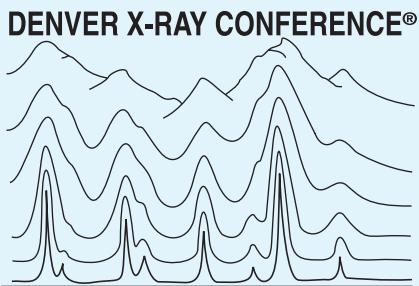
**Denise Zulli**, ICDD, Newtown Square, PA, [zulli@icdd.com](mailto:zulli@icdd.com)

## MEMBERS EMERITUS:

Victor Buhrke, Portola Valley, CA

Clay Ruud, Spokane, WA

## Future Conferences:



**31 July – 4 August 2017**

***Big Sky, Montana***

**6-10 August 2018**

***Westminster, Colorado***

# TABLE OF CONTENTS

## **WORKSHOPS**

---

<b>Monday Morning Workshops (9am - 12pm).....</b>	<b>Page 4</b>	<b>Tuesday Morning Workshops (9am - 12pm).....</b>	<b>Pages 6-7</b>
• Basic to Intermediate XRD I		• Structure Solution I	
• Diffraction Contrast Imaging		• Two-dimensional Detectors	
• Basic XRF		• Micro XRF	
• Synergies between Laboratory & Synchrotron X-ray Methods		• Quantitative Analysis I	
• Fundamentals of X-ray Absorption		• Amorphous & Disordered Materials I	
<b>Monday Afternoon Workshops (1:30pm - 4:30pm) ..</b>	<b>Page 5</b>	<b>Tuesday Afternoon Workshops (1:30pm - 4:30pm) ..</b>	<b>Page 7</b>
• Basic to Intermediate XRD II		• Structure Solution II	
• Rietveld for Beginners		• Advanced Rietveld	
• Energy Dispersive XRF		• XRF Sample Prep	
• Trace Analysis		• Quantitative Analysis II	
		• Amorphous & Disordered Materials II	

## **POSTER SESSIONS**

---

<b>Poster Sessions (5:00pm - 7:00pm)</b>	
• Monday XRD Poster Session.....	<b>Pages 8-10</b>
• Tuesday XRF Poster Session.....	<b>Pages 11-13</b>

## **ORAL SESSIONS**

---

<b>Wednesday Morning Session.....</b>	<b>Page 14</b>	<b>Thursday Afternoon Sessions.....</b>	<b>Pages 23-26</b>
• Plenary Session: Imaging at Current and Next Generation Synchrotrons		• Applied Materials I	
<b>Wednesday Afternoon Sessions.....</b>	<b>Pages 15-18</b>	• General XRD	
• High Energy X-ray Microscopy		• General XRF	
• Trace Analysis		• BioXRF: Related Techniques & Methods Development	
• BioXRF: Biomedical Applications		• X-ray Imaging II	
• New Developments in XRD & XRF Instrumentation I		<b>Friday Morning Sessions .....</b>	<b>Pages 27-29</b>
• X-ray Imaging I		• Stress	
<b>Thursday Morning Sessions .....</b>	<b>Pages 19-22</b>	• Applied Materials II	
• Rietveld		• Quantitative Analysis	
• Industrial Applications of XRF		• X-ray Optics	
• BioXRF: Plant/ Environmental/Microbial Science			
• New Developments in XRD/XRF Instrumentation II			
• Cultural Heritage			

## **PROGRAM-AT-A-GLANCE**

---

<b>Program-At-A-Glance.....</b>	<b>Page 30</b>
---------------------------------	----------------

## 2016 Denver X-ray Conference Workshops

MORNING WORKSHOPS – 9:00 AM – 12 NOON

AFTERNOON WORKSHOPS – 1:30 PM – 4:30 PM

MONDAY MORNING WORKSHOPS 9:00 AM – 12:00 NOON

### Basic to Intermediate XRD I

Lasalle C

Organizer & Instructors:

**M. Rodriguez**, Sandia National Laboratory, Albuquerque, NM, USA, marodri@sandia.gov

**T. Blanton**, ICDD, Newtown Square, PA, USA, tblanton@icdd.com

**S.T. Misture**, New York State College of Ceramics at Alfred University, Alfred, NY, USA, misture@alfred.edu

This workshop will discuss the use of XRD for standard qualitative analysis and will detail progressively more challenging means of XRD characterization including: quantitative analysis, profile fitting, lattice parameter refinement, crystallite size and microstrain determination, texture analysis, and structure refinement (Rietveld). Additionally, some discussion shall be dedicated to characterization of nanomaterials and glasses via pair distribution function analysis, as well as thin film techniques such as grazing incidence XRD and X-ray reflectivity (XRR). The workshop is intended to be a survey for the new user of XRD regarding what experiments can be performed and why one would wish to pursue such measurements.

### Diffraction Contrast Imaging

Madison

Organizer & Instructors:

**B. Patterson, D. Brown**, Los Alamos National Laboratory, Los Alamos, NM, bpatterson@lanl.gov; dbrown@lanl.gov

**J.S. Park**, Argonne National Laboratory, Argonne, IL, parkjs@aps.anl.gov

**E. Lauridsen**, Xnovo Technology, Køge, Denmark, info@xnovotech.com

This workshop will focus on using both synchrotron-based and laboratory-based instrumentation to understand the 3D crystallographic structure of materials. In situ measurements of polycrystalline materials, their starting morphologies, and their crystallographic response to stimuli (stress, thermal, radiation) can all be understood. The availability of these techniques in both synchrotron and laboratory based sources opens up a wide variety of X-ray techniques and allows researchers to customize the measurements for the materials of interest.

### Basic XRF

Lasalle A

Organizer & Instructors:

**A.R. Drews**, Ford Motor Company, Dearborn, MI, adrews@ford.com

**G.J. Havrilla**, Los Alamos National Laboratory, Los Alamos, NM, havrilla@lanl.gov

This workshop provides a basic introduction to the principles of XRF specifically aimed at those new to the field. In the first half, there will be a general overview of the XRF technique, including a discussion of the basic principles. The emphasis in the first half will be on understanding the underlying physical phenomena, how the technique is applied, optimization of the signal, and approaches to quantitative analysis. In the second half of the workshop, examples of real-world applications will be presented to illustrate some of the challenges and opportunities that the analyst may face. This half will describe a variety of specimen formats and demonstrate the flexibility of the XRF technique.

### Synergies between Laboratory and Synchrotron X-ray Methods

Lasalle B

Organizer & Instructors:

**G. Seidler**, University of Washington, Seattle, WA, USA, seidler@uw.edu

**U.E.A. Fittschen**, Washington State University, Pullman, WA, USA

**J. Cutler**, Canadian Light Source, Saskatoon, Canada

**S. Lapidus**, Argonne National Laboratory, Argonne, IL, USA

**M. Bedzyk**, Northwestern University, Evanston, IL, USA

Multiple speakers will address important industrial and basic research X-ray applications that span laboratory and synchrotron facilities. This will include XAFS, very high-resolution XRF for speciation, XRF imaging, powder XRD, and the much-improved integration of lab and synchrotron studies thanks to flexible rapid access scheduling, mail-in services, and on-site consultation.

### Fundamentals of X-ray Absorption Spectroscopy

Lakeshore A

Organizer & Instructors:

**G. Bunker, C. Segre**, Illinois Institute of Technology Physics Department, Chicago, IL, USA, bunker@iit.edu; segre@iit.edu

This workshop will provide an introductory overview of X-ray Absorption Fine Structure Spectroscopy for the study of the structures of materials. Applications to materials research will be described, and there will be an opportunity for Q&A. The workshop will conclude with an overview of some potential pitfalls and how to avoid them.

## MONDAY AFTERNOON WORKSHOPS 1:30 PM – 4:30 PM

### Basic to Intermediate XRD II

Lasalle C

Continued from Monday morning

### Rietveld for Beginners - Introduction to Rietveld fitting with GSAS-II

Lakeshore A

Organizers & Instructors:

**B. Toby, R. Von Dreele**, Argonne National Laboratory, Argonne, IL, USA, brian.toby@anl.gov; vondreele@anl.gov

This workshop will introduce basic concepts in Rietveld fitting and show how armed with an approximate crystal structure and a diffractogram, fitting is done with GSAS-II. Attendees will use their own laptops to fit an example set of data. Prerequisite: bring a laptop (Windows, Linux or Mac) with GSAS-II already installed (see <http://tinyurl.com/gsasii>).

### Energy Dispersive XRF

Lasalle A

Organizer & Instructors:

**P. Lemberge**, Thermo Scientific, Ecublens, Switzerland, pascal.lemberge@thermofisher.com

**R. Phillips**, Thermo Scientific, West Palm Beach, FL, rich.phillips@thermofisher.com

This workshop is designed to provide a discussion of the theoretical and practical aspects of EDXRF spectrometry providing a comprehensive review of the basic fundamentals for both the beginner and experienced X-ray spectroscopist. Topics to be covered include excitation systems; detectors; components and their relation to EDXRF applicability; ease of use; rapid qualitative analysis and material screening; calibration techniques for quantitative analysis; standard-less analysis; sensitivity of EDXRF for a wide variety of elements in various matrices as well as sample preparation. We discuss some real-life application examples where EDXRF is being used to solve complex analytical problems. The major emphases will be on the applicability of EDXRF and the optimal protocol for generating and reporting of reliable experimental results.

### Trace Analysis

Lasalle B

Organizers & Instructors:

**C. Streli, P. Wobraushek**, Vienna University of Technology, Vienna, Austria, streli@ati.ac.at; wobi@ati.ac.at

**K. Tsuji**, Osaka City University, Osaka, Japan, tsuji@a-chem.eng.osaka-cu.ac.jp

**N. Kawahara**, Rigaku Corporation, Osaka, Japan, kawahara@rigaku.co.jp

Both beginners and experienced X-ray physicists should gain information by attending the Trace Analysis workshop. Presentations of most modern techniques and instrumentation for trace element analysis using EDXRS will be given. Physical methods to improve minimum detection limits in XRF by background reduction will be discussed; special emphasis will be on synchrotron radiation as excitation source. Introduction to total reflection XRF (TXRF) and actual instrumentation will show achievable advantages and results in terms of detection limits, sensitivities and detectable elemental range down to light elements (eg. Carbon). Confocal  $\mu$ -XRF will be presented as method for 2D and 3D spatial resolved elemental imaging. Applications from interesting scientific fields as environment, microelectronics, forensic, and life science will show the successful use of the various XRF spectrometric techniques. The possibilities of trace analysis using wavelength dispersive XRF will also be covered, showing the benefits and limitations of the technique. A comparison of achievable detection limits with the various techniques on some specific samples will be discussed.

## TUESDAY MORNING WORKSHOPS 9:00 AM – 12:00 NOON

### Structure Solution I

Madison

#### Organizers & Instructors:

**J. Kaduk**, Poly Crystallography Inc. and Illinois Institute of Technology, Naperville, IL, USA, Kaduk@polycrystallography.com

**R. Papoula**, Saclay Institute for Matter and Radiation (IRAMIS), LLB, CEA-Saclay, France, robert.papoula@cea.fr

This workshop addresses beginners and those of intermediate experience. The background of the principal methodologies for structure solution using powder data (direct methods, charge flipping, and real space methods such as Monte Carlo simulated annealing and parallel tempering) will be discussed, but the main focus of the workshop will be hands-on practice in solving structures using laboratory, synchrotron, and neutron powder data. We encourage the attendees to bring their own computers with EXPO2014, Jana2006, GSAS-II, and FOX already installed.

### Two-dimensional Detectors

Lakeshore A

#### Organizers & Instructors:

**T. Blanton**, ICDD, Newtown Square, PA, USA, tblanton@icdd.com

**B. He**, Bruker AXS, Inc., Madison, WI, USA, bob.he@bruker.com

Two-dimensional diffraction data contains abundant information about the atomic arrangement, microstructure, and defects of a solid or liquid material. In recent years, the use of two-dimensional detectors has dramatically increased in academic, government and industrial laboratories. This workshop covers recent progress in two-dimensional X-ray diffraction in terms of detector technology, geometry, and configuration of the two-dimensional diffractometer. Various applications such as phase ID, texture, stress, crystallinity, combinational screening, and thin film analysis will be discussed.

### Micro XRF

Lasalle A

#### Organizer & Instructors:

**G.J. Havrilla**, Los Alamos National Laboratory, Los Alamos, NM, havrilla@lanl.gov

**A. Lanzirotti**, The University of Chicago – CARS, Argonne, IL, USA, lanzirotti@uchicago.edu

The MXRF workshop will provide an overview of micro X-ray fluorescence for solving analytical problems. This overview will include X-ray optics used in MXRF, capabilities, survey of commercial instrumentation, and confocal and monochromatic wavelength dispersive XRF. The workshop will cover “how to” guidelines for applying laboratory-based and synchrotron source MXRF, as well as unique capabilities and applications for each excitation source.

### Quantitative Analysis I

Lasalle B

#### Organizer & Instructors:

**W.T. Elam**, University of Washington, Seattle, WA, wtelam@apl.washington.edu

**B. Vrebos**, PANalytical B.V., Almelo, The Netherlands, bruno.vrebos@panalytical.com

**K. Kawakyu**, Rigaku Corporation, Osaka, Japan, kawakyu@rigaku.co.jp

- Morning: Source of matrix effects and scatter peaks, compensation methods, semi-quantitative analysis using FP, and fusion
- Afternoon: Introduction to mathematics and physics of XRF quantification

### Amorphous & Disordered Materials I

Lasalle C

#### Organizer & Instructors:

**T. Fawcett**, ICDD, Newtown Square, PA, USA, fawcett@icdd.com

**S. Bates**, Triclinic Labs, Inc., West Lafayette, IN, USA, sbates@tricliniclabs.com

**M. Leoni**, University di Trento, Trento, Italy, Matteo.Leoni@unitn.it

**A. Newman**, Seventh Street Development Group, Lafayette, IN, USA, ann.newman@seventhstreetdev.com

**V. Petkov**, Central Michigan University, Mt. Pleasant, MI, USA, petko1vg@cmich.edu

#### **Morning (9:00am - 12:00pm)**

This workshop will discuss the various methods and techniques used to make amorphous materials. We will then discuss the basics of amorphous materials, solid dispersions, disordered structures, and nanomaterials. Finally, we will cover the structural basis of amorphous materials and the use of diffraction methods for characterization.

Topics include:

- Making amorphous materials
- Amorphous and amorphous solid dispersions
- How are amorphous materials defined
- Amorphous materials: A structural perspective
- The use of powder diffraction

## **Afternoon (1:30pm - 4:30pm)**

In this workshop, we will discuss the various diffraction methods used to elucidate the physical nature of amorphous and disordered materials. This will include overviews of the most frequently used techniques and tools such as full pattern analyses, line profile analyses, and pair distribution functions. The intent is not to cover these subjects in full detail, each could be a separate workshop, but to present a comprehensive look at the available tools.

Topics include:

- The analysis of amorphous and disordered materials by full pattern methods
- The analysis of microstructure by line profile analysis
- The analysis of microstructure by atomic pair distribution analysis

## **TUESDAY AFTERNOON WORKSHOPS 1:30 PM – 4:30 PM**

### **Structure Solution II**

**Madison**

Continued from Tuesday morning.

### **Advanced Rietveld - Advanced use of GSAS-II**

**Lakeshore A**

Organizers & Instructors:

**B. Toby, R. Von Dreele,** Argonne National Laboratory, Argonne, IL, USA, brian.toby@anl.gov; vondreele@anl.gov

This workshop will provide an overview of some of the sophisticated and unique capabilities in GSAS-II such as (1) area detector calibration, integration and automated data reduction, (2) indexing and structure solution from powders, (3) combined refinements and (4) parametric analysis, as well as providing information on what are the latest developments and what is coming soon. Attendees will select a set of tutorials for one of the above topics to complete. Prerequisites: attendees are expected to have attended “Introduction to Rietveld fitting with GSAS-II” or to have already be familiar with basic use of GSAS-II; they are expected to also bring a laptop (Windows, Linux or Mac) with GSAS-II already installed (see <http://tinyurl.com/gsasii>).

### **Sample Preparation of XRF**

**Lasalle A**

Organizer & Instructors:

**J. Anzelmo,** Anzelmo & Associates, Inc., Madison, WI, jaanzelmo@aol.com

**M. Provencher,** Corporation Scientifique Claisse, Quebec City, Quebec, Canada, maprovencher@claisse.com

This workshop will begin with John Anzelmo discussing the fundamental physics of sample preparation, such as infinite thickness and effective layer thickness, particle size effects, mineralogical effects, grinding concepts, and how to make the basic laboratory operations involved in solving these problems for XRF specimen preparation of pressed powders and fusion beads. Marie-Ève Provencher will discuss basic and advanced fusion techniques, such as selection of flux for different applications, conditions that cause cracking in beads, and oxidation techniques for simple and difficult to flux materials.

### **Quantitative Analysis II**

**Lasalle B**

Continued from Tuesday morning.

### **Amorphous & Disordered Materials II**

**Lasalle C**

Continued from Tuesday morning.

## XRD Poster Session – Monday Evening, Michigan Room

The Monday Evening XRD Poster Session will be held 5:00 PM – 7:00 PM in the Michigan Room, in conjunction with a Wine & Cheese Reception.

Three “Best Poster” awards will be given at the end of the session, including “Best Student Poster”.

\*Signifies Presenting Author, when noted

- D-6 **X-ray Diffraction Study of Nanocellulose II Produced from the Amazonian Seed Coconut (Tucumã)**  
L. Manzato, IFAM, Manaus, AM, Brazil  
S.M. de Souza, UFAM, Manaus, AM, Brazil  
J. Simonsen, OSU, Corvallis, OR, USA
- D-8 **X-ray Analysis for Quantifying Various Components in Poly(vinyl chloride) Plastics**  
P. Ricou, R. Smith, Arkema Inc., King of Prussia, PA, USA
- D-11 **Structural Investigation of Chemical Ordering in the  $(\text{Ga}_{1-x}\text{Zn}_x)(\text{N}_{1-x}\text{O}_x)$  Visible-light Photocatalyst by Neutron and X-ray Diffraction**  
D. Chen\*, S. Skrabalak, Indiana University, Bloomington, IN, USA
- D-12 **Phase Equilibria in the Co-Fe-Si Ternary System using Synchrotron Powder Diffraction**  
J. Hasier, I.M. Hawgood, P. Nash, Illinois Institute of Technology, Chicago, IL, USA
- D-16 **What Is the Origin of a Series of Low Angle XRD Peaks Which Appear Following Thermal Cycling of a Gadolinium - Doped Ceria Film – Formation of a Superlattice or Surface Contamination?**  
Y. Feldman\*, I. Zon\*, Weizmann Institute of Science, Rehovot, Israel  
V. Shelukhin, Tel-Aviv University, Tel-Aviv, Israel
- D-18 **Operando XRD-DRIFT: Catalyst Characterization by Fisher-Tropsch Process for Clean Fuel Production**  
C. Fontugne, Thermo Scientific, Artenry, France  
V. Moizan-Basle, L. Braconnier, I. Clemenccon, C. Legens, B. Robours, L. Lemaitre, IFP, Lyon, France
- D-22 **Crystallographic Studies of Solvent Sorption in a Flexible 2D Layer Spin Crossover Coordination Polymer**  
Y.-C. Chuang\*, C.-K. Chang, J.-J. Lee, National Synchrotron Radiation Research Center, Hsinchu, Taiwan  
C.-C. Wang, Soochow University, Taipei, Taiwan
- D-23 **Analysis of Steels by Handheld XRD**  
G.M. Hansford, University of Leicester, Leicester, UK
- D-24 **Synchrotron Powder Diffraction Simplified: The High-Resolution Diffractometer 11-BM at the Advanced Photon Source**  
L. Ribaud\*, S. Lapidus, R. Von Dreele, B. Toby, Argonne National Laboratory, Argonne, IL, USA
- D-26 **Stacking Faults and Phase Transformations Study in Ball Milled  $\text{Co}_{100-x}\text{Cr}_x(x = 0, 20, 50)$  Alloys**  
S. Louidi, University 20 Août-1955, Skikda, Algeria  
F.-Z. Bentayeb, Université Badji-Mokhtar, Annaba, Algeria  
J.J. Sunol, Universitat de Girona, Girona, Spain
- D-28 **The Mineralogy, Nucleation and Growth of Freshwater Ferromanganese Nodules**  
S. Lee, H. Xu\*, NASA Astrobiology Institute, University of Wisconsin –Madison, Madison, WI, USA
- D-29 **The Influence of the Sintering Temperature and Synthesis Method on the Structural Properties of Doped Perovskites Like:  $\text{La}_{0.75}\text{Sr}_{0.25}\text{Cr}_{0.5-0.7}\text{Fe}_{0.5-0.3}\text{O}_3$  (LSCF) And  $\text{BaZr}_{0.7}\text{Pr}_{0.1}\text{Y}_{0.2}\text{O}_3$  (BZPY)**  
K. Küçük\*, A. Coskun, A.S. Hock, C.U. Segre, Illinois Institute of Technology, Chicago, IL, USA
- D-31 **Extended Range Ultra Small-Angle, Small-Angle, and Wide-Angle X-ray Scattering Facility for Materials Development**  
J. Ilavsky\*, R. Andrews, APS, Argonne National Laboratory, Lemont, IL, USA  
G. Muralidharan, Oak Ridge National Laboratory, Oak Ridge, TN, USA  
F. Zhang, L.E. Levine, A.J. Allen, National Institute of Standards and Technology, Gaithersburg, MD, USA

- D-36 A Study on Correlation of Electrochemical Behavior with Structural Defects in Olivine System**  
**Y. Kim, J. Yoo, M. Jeong, W.-S. Yoon**, Sungkyunkwan University, Suwon, Gyeonggi-do, South Korea  
**N.-H. Lee**, Umicore Korea Limited, Cheonan, Gyeonggi-do, South Korea
- D-38 STOE InSitu HT2 – A New In Situ Reaction Chamber in Debye-Scherrer Geometry**  
**T. Hartmann**, Stoe & Cie GmbH, Darmstadt, Germany
- D-41 Hydrogen Production from Oxidative Steam Reforming of Ethanol on Pyrochlore Phase Materials Contains Nickel**  
**H.-C. Hsieh, S.-F. Weng, C.-S. Lee**, National Chiao-Tung University, Hsinchu, Taiwan  
**J.-F. Lee, H.-S. Sheu**, National Synchrotron Radiation Research Center, Hsinchu, Taiwan
- D-42 Crystal Structures and Properties of New Compounds in  $MgO-In_2O_3-P_2O_5$  Ternary Systems**  
**J. Zhang, G. Cai, Z. Jin**, Central South University, Changsha, China
- D-43 Structural Characterization of Perovskite-Based Photovoltaics by X-ray Diffraction Analysis**  
**H.F. Garces, Y. Zhou, N.P. Padture**, Brown University, Providence, RI, USA
- D-46 Recent Developments on Incoatec's Microfocus Source I $\mu$ S**  
**B. Hasse, A. Kleine, J. Graf, C. Michaelsen**, Incoatec GmbH, Geesthacht, Germany
- D-47 Crystal Structures of Large-Volume Commercial Pharmaceuticals**  
**J.A. Kaduk**, Illinois Institute of Technology, Chicago, IL, USA and North Central College, Naperville, IL, USA  
**R.J. Papoulier**, IRAMIS/CEA - Saclay, Gif-sur-Yvette Cedex, FRANCE  
**A.M. Gindhart, T.N. Blanton**, ICDD, Newtown Square, PA, USA
- D-49 The Use of ' $\alpha$ '-Reflections in Determining the Dolomite Ordering State**  
**F. Hobbs\***, H. Xu, University of Wisconsin-Madison, Madison, WI, USA
- D-51 X-ray Analysis of Size and Size Distribution of  $Fe_3O_4$  Magnetic Nano-Particles**  
**J. Li**, Rice University, Houston, TX, USA
- D-53 Quartz: Structural and Thermodynamic Analyses Across the  $\alpha \leftrightarrow \beta$  Transition with Origin of Negative Thermal Expansion (NTE) in  $\beta$  Quartz and Calcite**  
**S.M. Antao**, University of Calgary, Calgary, Alberta, Canada
- D-56 USAXS-SAXS-WAXS Characterization of Coarsening in Nickel Alloys**  
**R. Andrews, J. Ilavsky**, Argonne National Laboratory, Lemont, IL, USA  
**G. Muralidharan**, Oak Ridge National Laboratory, Oak Ridge, TN, USA
- D-58 XRD Characterization of Luminescent and Magnetic Nanoparticles Synthesized by Sol-Gel Proteic and Starch-Gel Methods**  
**G. Lopes, M. Santos, J. Nascimento, F. Costa, A. Souza, S. Batista, T. Souza**, State University of Amapá, Macapá, AP, Brazil
- D-64 Powder XRD and TEM Study on Structures, Stacking Faults, and Interstratification in Cu-Chlorite and Zn-Chlorite (Baileychlore)**  
**H. Xu**, University of Wisconsin-Madison, Madison, WI, USA
- D-69 Further Results of X-ray Diffraction of Nuclear Forensic Samples**  
**S. Roberts**, Lawrence Livermore National Laboratory, Livermore, CA, USA
- D-72 Synthesis of  $MnO_2$  Nanomaterials with Fine Control of Morphology and Crystalline Phase Composition**  
**E. Moazzen, E. Timofeeva, C. Segre**, Illinois Institute of Technology, Chicago, IL, USA
- D-75 Optimization of Temperature Measurement in the TTK 600 Low-Temperature Chamber and BTS 150/500 Benchtop Heating Stage**  
**B. Puhr\***, Anton Paar GmbH, Graz, Austria
- D-76 Local Structure of Amorphous Indometacin Studied with X-ray Total Scattering Analysis using Bench-Top Diffractometer**  
**J. Rantanen\*, V-P Lehto**, University of Eastern Finland, Kuopio, Finland

- D-77 Fe-Treated Heteroatom-Doped Graphene as New Catalysts for Water Oxidation**  
F. Razmjooei, K.P. Singh, J.-S. Yu, DGIST, Daegu, Korea
- D-78 Structural Study in Cu<sub>x</sub>Co<sub>1-x</sub>Fe<sub>2</sub>O<sub>4</sub> And Cu<sub>x</sub>Mg<sub>1-x</sub>Fe<sub>2</sub>O<sub>4</sub> Spinnels**  
S. Ouyahia, K. Taibi, A. Rais, USTHB, Algiers, Algeria
- D-80 JATOBÁ Beamline - High Energy In Situ X-ray Diffraction**  
L. Wu, E.B. Fonseca, A.P. Tschiptschin, Brazilian Nanotechnology National Laboratory, Campinas, SP, Brazil  
H. Westfahl Jr, Brazilian Synchrotron Light Laboratory, Campinas, SP, Brazil  
G. Faria, Ohio State University, Columbus, OH, USA
- D-83 Reciprocal Space Mapping Study of CdTe Epilayer Grown by Molecular Beam Epitaxy on (211)B GaAs Substrate**  
M. Polat\*, O. Ari, O. Öztürk, Y. Selamet, Izmir Institute of Technology, Izmir, Turkey
- D-87 Complementary SAXS, PDF, and XRD Analysis of Quantum Dots**  
S. Speakman, PANalytical, Westborough, MA, USA
- D-91 Certification of SRM 1979; Line Profile Standard for Analysis of Crystallite Size**  
J.P. Cline, M.H. Mendenhall, J.J. Ritter, D. Black, A. Henins, J.E. Bonevich, NIST, Gaithersburg, MD, USA  
P. Whitfield, Oak Ridge National Laboratory, Oak Ridge, TN, USA
- D-92 A High-Precision Measurement of the Cu K $\alpha$  Emission Spectrum**  
M.H. Mendenhall, J.P. Cline, A. Henins, L.T. Hudson, C.I. Szabo, D. Windover, NIST, Gaithersburg, MD, USA
- D-94 ICDD Full Diffraction Pattern Polymer Project – New Entries for PDF-4+ 2016 and PDF-4 Organics 2017**  
T. Blanton, S. Gates, ICDD, Newtown Square, PA, USA  
S. Misture, Alfred University, Alfred, NY, USA
- D-95 Improvements in Benchtop Powder Diffraction Utilizing PROTO's AXRD Diffractometer**  
N. Vukotic\*, M. Belassel, PROTO, Oldcastle, ON, Canada  
W. Boyer, PROTO, Taylor, MI, USA
- D-97 Characterization of NiAl Thin Films Using SmartLab Diffractometer**  
N. Anibou, Rigaku Americas, The Woodlands, TX, USA  
W. Donner, Technische Universität Darmstadt, Darmstadt, Germany
- D-102 Computer Simulation for the Lattice Expansion In Delta Plutonium**  
C. Saw, Lawrence Livermore National Lab, Livermore, CA, USA
- D-105 Microstructural Characterization of Fly Ash-based Geopolymer**  
Y. Ling\*, K. Wang, Iowa State University, Ames, IA, USA  
S. Hua, Nanjing Technology University, Nanjing, Jiangsu, China  
J. Liu, Jiangsu Research Institute of Building Science, Nanjing, Jiangsu, China
- S-11 Using Radial Distribution Function to Analyze the Structure of Indium Oxide**  
T. Bsaibes, DePaul University, Chicago, IL, USA  
G.B. Gonzalez Aviles, DePaul University, Chicago, IL, USA
- S-16 Characterization of Thin Diamond Crystals for X-ray Split and Delay Line**  
P. Vodnala\*, L.B. Lurio, Northern Illinois University, Aurora, IL, USA  
T. Kolodziej, S. Stoupin, Y.V. Shyvd'ko, Argonne National Laboratory, Argonne, IL, USA  
S. Terentyev, V. Blank, Technological Institute for Superhard and Novel Carbon Materials, Troitsk, Russian Federation
- S-17 Effect of Zinc and Strontium Dopants on the Structure and Stability of Hydroxyapatite at High Temperatures**  
D. Smith\*, G. Gonzalez Aviles, DePaul University, Chicago, IL, USA
- S-35 In Situ EXAFS Studies of MoS<sub>2</sub> for Li-ion Batteries**  
N. Beaver, S. Aryal, J. Katsoudas, E. Timofeeva, C. Segre, Illinois Institute of Technology, Chicago, IL, USA
- S-36 XRD and In Situ XAS Study of Cycled Core/Shell Ni(OH)<sub>2</sub>/Co(OH)<sub>2</sub> Nanoparticles for Battery Cathodes**  
E. Moazzen, E. Timofeeva, C. Segre, Illinois Institute of Technology, Chicago, IL, USA

## XRF Poster Session – Tuesday Evening, Michigan Room

The Tuesday Evening XRF Poster Session will be held 5:00 PM – 7:00 PM in the Michigan Room, in conjunction with a Wine & Cheese Reception.

Three “Best Poster” awards will be given at the end of the session, including “Best Student Poster”.

\*Signifies Presenting Author, when noted

- F-2 Archaeological Characterization of Ancient Pottery from Izu Islands (Tokyo, Japan) by Chemical Compositions Obtained from XRF**  
S. Ichikawa\*, T. Nakamura, Meiji University, Kawasaki, Kanagawa, Japan  
T. Matsumoto, Tokai University, Hiratsuka, Kanagawa, Japan
- F-6 Method Development for the Quantification of Dissolved Major Components of Radioactive Liquid Waste**  
T. Ely, G. Cooke, Washington River Protection Solutions LLC, Richland, WA, USA
- F-7 Laboratory-typed Polychromatic XRF for Chemical State Analysis using Silicon Strip Detector and Laboratory X-ray Source**  
K. Sato\*, A. Nishimura, M. Kaino, S. Adachi, Shimadzu Corporation, Kyoto, Japan
- F-8 Content Distribution Analysis of Nb, Ti, Mo, W in Superalloys by High-resolution XRF Scanning Method**  
D.L. Li, L. Zhao, L.X. Yang, H.Z. Wang, Central Iron & Steel Research Institute, Beijing, China
- F-11 Multiscale Analysis of Cu in 9Cr-3W-3Co Martensitic Heat Resistant Steels for Ultra-supercritical Power Plants by Micro-XRF/ EDS on SEM**  
L.X. Yang, L. Zhao, D.L. Li, X.J. Li, H.Z. Wang, China Iron & Steel Research Institute, Beijing, China
- F-18 X-ray Reflectometry Study of the Structures of Langmuir-Schaeffer Films of Encapsulated Nanoparticles**  
N. Al-Senany, King Abdulaziz University, Jeddah, Saudi Arabia  
T. Richardson, N. Cowlam, University of Sheffield, Sheffield, UK
- F-19 Comparison Between Different Quantification Methods in the EDXRF Analysis of Precious Alloys**  
F. Niccolai, A. Amato, J. Ravagli, Sinerlab S.r.l., Quarrata (PT), Italy  
S. Gonzi, University of Florence, Firenze, Italy  
D.M. Musale, Quantum Equipment Co. Pvt. Ltd., Mumbai, India  
S. Ridolfi\*, Ars Mensurae, Roma, Italy
- F-20 On-Site Determination of Heavy Metals in Water Using Handheld X-ray Fluorescence Spectrometer**  
K. Hagiwara, S. Kai, Y. Koike, M. Aizawa, T. Nakamura, Meiji University, Kawasaki, Kanagawa, Japan
- F-21 Safety Handling of Handheld X-ray Fluorescence Spectrometer Based on Determination of Two-dimensional Imaging of Scattering Radiation**  
K. Fujii, K. Hagiwara, W. Matsuda, T. Nakamura, Y. Koike, Meiji University, Kawasaki, Kanagawa, Japan
- F-22 The Synchrotron X-ray Study on the Reaction Mechanism of Metal Oxide Based Anode Materials with High Abnormal Capacity for Lithium-Ion Batteries**  
H. Kim, J. Yoo, Y. Kim, W.-S.Yoon, Sungkyunkwan University, Suwon, Gyeonggi-do, South Korea  
M. Balasubramanian, Argonne National Laboratory, Lemont, IL, USA
- F-23 Large Area 7-Channel Silicon Drift Detector Array**  
A. Pahlke, R. Fojt, M. Fraczek, M. Hofmann, L. Hoellt, J. Knobloch, E. Lechner, N. Miyakawa, S. Pahlke, J. Rumpff, O. Scheid, A. Simsek, R. Stoetter, KETEK GmbH, Munich, Germany
- F-24 Calculation of Fluorescent X-ray Intensity Calculation for Confocal Micro-XRF Analysis of Inhomogenous Samples**  
N. Kawahara\*, T. Matsuno, K. Tsuji, Osaka City University, Osaka, Japan
- F-27 Application of Metal Impurity Trace Analysis in Pharmaceutical Materials Using Unique FP Method for Assessment Elements Based on ICH Q3D**  
H. Furukawa, N. Ichimaru, H. Ochi, Shimadzu Corporation, Kyoto, Japan  
D. Davis, Shimadzu Scientific Instruments, Inc., MD, USA  
C. Yomota, Pharmaceutical and Medical Device Regulatory Science Society of Japan, Osaka, Japan

- F-36 Environmental Sample Examples by Portable Reflection X-ray Fluorescence Spectrometer**  
J. Kawai\*, Kyoto University, Kyoto, Japan  
H. Nagai, Y. Nakajima, Ourstex, Osaka, Japan
- F-39 Analyzing Absorption of Wood Preservatives Using Micro-X-ray Fluorescence**  
A. Lee, B. Scruggs, Edax, Mahwah, NJ, USA
- F-47 The Development of TXRF Method and its Application on the Study of Trace Elements in Water at SSRF**  
L. Wang, H. Yu, L. Li, X. Wei\*, Y. Huang\*, Chinese Academy of Sciences, Shanghai, China
- F-56 Multi-Element Silicon Drift Detectors for High Speed X-ray Spectroscopy and Mapping Applications**  
M. Zhang, S. Barkan, V.D. Saveliev, Y. Wang, L. Feng, B. Goolsby, E.V. Damron, Y. Tomimatsu, Hitachi High-Technologies Science America, Inc., Northridge, CA, USA  
R. Goldsbrough, Quantum Detectors Ltd., Harwell, Oxford, UK
- F-57 Elemental Characterization of Airborne Particulate Matter Collected within IMPROVE and CSN Networks**  
K. Trzepla \*, S. Yatkin, W. White, N. Hyslop, University of California, Davis, CA, USA
- F-58 X-ray Fluorescence Measurements of Pharmaceutical Sprays**  
D. Duke\*, A. Kastengren, Argonne National Laboratory, Lemont, IL, USA  
N. Mason-Smith, D. Edgington-Mitchell, D. Honnery, Monash University, Melbourne, VIC, Australia
- F-59 Investigation of Heavy Metal Deposition in Zebrafish by Total Reflection X-ray Fluorescence**  
M. Schmeling, J. Arroyo, R. Dale, E. Jamka, K. Niaz, Loyola University Chicago, Chicago, IL, USA
- F-60 Quantification of Nanoparticles Used in Biomedical Applications via Total Reflection X-ray Fluorescence**  
G. Mankovskii \*, E. Da Silva, J. Grafe, A. Pejovic-Milic, Ryerson University, Toronto, Ontario, Canada
- F-62 Increased Zinc Accumulation in Mineralized Osteosarcoma Tissue Measured by SR- $\mu$ XRF Analysis**  
M. Rauwolf, B. Pemmer, A. Turyanskaya, S. Smolek, A. Maderitsch, P. Hischenhuber, C. Weixelbaumer, M. Foelser, P. Wobrauscheck, C. Streli\*, Atominstutit TU Wien, Vienna, Austria  
A. Roschger, K. Klaushofer, P. Roschger, J.G. Hofstaetter, Hanusch Hospital of WGKK and AUVA Trauma Centre Meidling, Vienna, Austria  
R. Simon, Karlsruhe Institute of Technology (KIT), ANKA synchrotron radiation source, Karlsruhe, Germany  
S. Lang, S. E. Puchner, R. Windhager, Vienna General Hospital, Medical University of Vienna, Vienna, Austria
- F-63 Zn Distribution in Healing Osteoporotic Fractures Measured by SR- $\mu$ XRF Analysis**  
M. Rauwolf, A. Turyanskaya, B. Pemmer, J. Prost, P. Wobrauscheck, C. Streli\*, Atominstutit TU Wien, Vienna, Austria  
A. Roschger, K. Klaushofer, P. Roschger, J.G. Hofstaetter, Hanusch Hospital of WGKK and AUVA Trauma Centre Meidling, Vienna, Austria  
R. Simon, Karlsruhe Institute of Technology (KIT), ANKA synchrotron radiation source, Karlsruhe, Germany  
I. Pape, Diamond Light Source Ltd, Oxfordshire, UK
- F-64 SR-TXRF-XANES of Indoor Aerosol Samples at BESSYII and ELETTRA**  
J. Prost, A. Windbichler, P. Wobrauscheck, C. Streli, Atominstutit, TU Wien, Vienna, Austria  
A. Guilherme Buzanich, U. Reinholtz, H. Riesemeier, M. Radtke, Institute for Materials Research and Testing (BAM), Berlin, Germany  
G. Pepponi, MiNaLab, CMM-irst, Fondazione Bruno Kessler, Trento, Italy  
A. Migliori, A.G. Karydas, M. Czyzycki, IAEA, Seibersdorf, Austria  
D.M. Eichert, W.H. Jark, ELETTRA - Sincrotrone Trieste, Trieste, Italy
- F-65 Total Reflection X-ray Fluorescence Analysis of Indoor Aerosol Samples – Influence of Sampling Time and Comparison of Different Direct Sampling Methods**  
J. Prost, A. Windbichler, A. Zinkl, A. Hable, J.H. Sterba, P. Wobrauscheck, C. Streli, Atominstutit, TU Wien, Vienna, Austria  
A.G. Karydas, IAEA, Seibersdorf, Austria
- F-66 Manganese Distribution in Healthy and Osteoporotic Human Bone**  
A. Turyanskaya, M. Rauwolf, J. Prost, P. Hischenhuber, P. Wobrauscheck, C. Streli, TU Wien, Atominstutit, Vienna, Austria  
A. Roschger, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany  
A. Roschger, P. Roschger, J.G. Hofstaetter, K. Klaushofer, Hanusch Hospital of WGKK and AUVA Trauma Centre Meidling, Vienna, Austria  
J.G. Hofstaetter, Orthopaedic Hospital Vienna-Speising, Vienna, Austria  
R. Simon, Karlsruher Institute for Technology (KIT), ANKA Synchrotron Radiation Source, Karlsruhe, Germany

- F-67 Elemental Imaging on Biodegradable Orthopedic Implants by µXRF**  
A. Turyanskaya, M. Rauwolf, J. Prost, L. Pernezky, P. Wobrauschek, C. Streli, TU Wien, Atominstitut, Vienna, Austria  
T.A. Gruenewald, M. Meischel, H. Lichtenegger, S.E. Stanzl-Tschegg, University of Natural Resources and Life Sciences (BOKU), Vienna, Austria  
A.M. Weinberg, Medical University Graz, Graz, Austria
- S-14 Capping Layer Effects of Au and Al On Fe/(Ga,Mn) as Bilayers Studied by X-ray Absorption Spectroscopy**  
A.M. Alsmadi\*, Kuwait University, Kuwait, Kuwait  
Y. Choi, D.J. Keavney, Argonne National Laboratory, Argonne, IL, USA  
X. Liu, M. Dobrowolska, J.K. Furdyna, University of Notre Dame, Notre Dame, IN, USA  
K. Tivakornasithorn, Mahidol University, Bangkok, Thailand
- S-15 Micro-Computed Tomography for Morphometry of Non-Mineralized Fresh and Plastic Embedded Biological Tissues Subjected to Laser Ablation**  
A. Robinson, S. Stock, C. Richter, Northwestern University, Chicago, IL, USA  
C. Soriano, X. Xiao, Argonne National Laboratory, Argonne, IL, USA
- S-20 Using Statistical and Geostatistical Information to Identify Soil Particulate Organic Matter on X-ray Computed Micro-Tomography Images**  
A. Kravchenko, A. Guber, D. Colbry, Michigan State University, East Lansing, MI, USA
- S-22 EDX, Raman, Optical Microscopy and Multivariate Statistics Analysis of Archaeological Pottery from São Luiz, MA, Brazil**  
R. Ikeoka, C. Appoloni, O.H. Marcori, State University of Londrina - UEL, Londrina, PR, Brazil  
A.M. Bandeira, Universidade de São Paulo, São Paulo, SP, Brazil
- S-33 Time-Lapse Micro X-ray Computed Tomography Study of Moisture- and Mechanically-Induced Twisting of Wood Slivers**  
X. Arzola, R. Lakes, University of Wisconsin, Madison, WI, USA  
X. Xiao, APS, Argonne National Laboratory, Argonne, IL, USA  
J. O'Dell, J. Jakes, USDA Forest Service, Madison, WI, USA
- S-41 CaCO<sub>3</sub>: Probing the Complex Chemistry of a Simple and Ubiquitous Material with X-ray Absorption Spectroscopy**  
E.A. Willneff\*, T. Kathyola, P. Mougkogiannis, University of Leeds, Leeds, UK  
S.Y. Chang, Diamond Light Source, Oxford, UK
- S-42 Developments in Equilibrium and Time-Resolved Small Angle X-ray Scattering**  
S. Chakravarthy, T. Irving, BioCAT/Illinois Institute of Technology, Chicago, IL, USA  
S. Kathuria, O. Bilsel, U Mass. Medical School, Worcester, MA, USA
- S-44 Measuring Crystal Characteristics of Intact Archeological Human Second Metacarpal Bones as a Function of Individuals' Age at Death**  
S.R. Stock\*, Northwestern University, Chicago, IL, USA  
J.S. Park, J.D. Almer, Argonne National Laboratory, Argonne, IL, USA  
I.G. Nielsen, H. Birkedal, Aarhus University, Aarhus, DK  
S. Mays, English Heritage, Portsmouth, UK
- S-51 Synchrotron Radiation Studies of Multilayered ZrC/SiC Thin Films for Advanced Nuclear Fuel Cladding Applications**  
D. Velazquez\*, R. Seibert, W. Limestall, Z. Lee, J. Terry, Illinois Institute of Technology, Chicago, IL, USA
- S-52 Synchrotron Characterization of Fission Products in the SiC Containment Layer in High Burnup TRISO Fuel**  
R.L. Seibert\*, J. Terry, Illinois Institute of Technology, Chicago, IL, USA  
K. Terrani, F. Montgomery, C. Baldwin, K. Leonard, Oak Ridge National Laboratory, Oak Ridge, TN, USA
- S-59 Development of Low Cast X-ray Imaging for Solidification of Cast Steels**  
C. Chuang, D. Singh, P. Kenesei, J. Almer, J. Hryn, Argonne National Laboratory, Lemont, IL, USA

## Plenary Session – Wednesday Morning, 8:30 AM – 12:00 PM

Lasalle Ballroom

### Plenary Session: Imaging at Current and Next Generation Synchrotrons

Chair: **Brian Toby**, Argonne National Laboratory, Advanced Photon Source, Argonne, IL, USA

8:30

#### Opening Remarks & Awards:

Chairman of the Denver X-ray Conference, **W. Tim Elam**, University of Washington APL, Seattle, WA, USA

#### Presentation of Awards:

2016 Birks Award to be announced

2016 Jerome B. Cohen Student Award. The winner will be announced at the session.

Presented by **Cev Noyan**, Columbia University, New York, NY, USA

2016 Robert L. Snyder Student Travel Awards to be announced

2016 Hanawalt Award presented to **Matteo Leoni** and **Paolo Scardi**, University di Trento, Trento, Italy

Plenary Session remarks by the Session Chair, **Brian Toby**.

**Invited Talks** \*Signifies Presenting Author, when noted

9:00 D-106 100 Years of Powder Diffraction

**Tim Fawcett**, International Centre for Diffraction Data, Newtown Square, PA, USA

9:30 S-13 X-ray Imaging at the Advanced Photon Source (APS) from Data Intensive to Data Driven: Opportunities with the APS Upgrade

**F. De Carlo\***, **V. De Andrade**, **K. Fezzaa**, **T. Sun**, **X. Xiao**, Argonne National Laboratory, Argonne, IL, USA

10:15 Break

10:45 F-69 X-ray Fluorescence Microscopy: Advances and Unique Opportunities

**Stefan Vogt\***, **S-C. Gleber**, **D. Vine**, **S. Chen**, **L. Finney**, **O. Antipova**, **L.X. Li**, **B. Lai**, APS, Argonne National Laboratory, Argonne, IL, USA

**B. Twining**, Bigelow Laboratory, East Boothbay, USA

**S. Baines**, Stony Brook University, Stony Brook, NY, USA

**C. Fahrni**, **D. Bourassa**, **E. Ingall**, Georgia Institute of Technology, Atlanta, GA, USA

**J. Deng**, Northwestern University, Chicago, IL, USA

**C. Jacobsen**, APS, Argonne National Laboratory, Argonne, IL, USA and Northwestern University, Chicago, IL, USA

**J.E. Jakes**, **C.G. Hunt**, **D.J. Yelle**, **C. Preissner**, Forest Products Laboratory, Madison, WI, USA

11:30 Hanawalt Award Lecture: Detailed Microstructure Information from Powder Data: A Maze or Amazing?

**Matteo Leoni**, University di Trento, Trento, Italy

Note: **Paolo Scardi** will present his Hanawalt Award Lecture at the **15th European Powder Diffraction Conference (EPDIC15)**, being held in Bari, Italy, 12 - 15 June 2016.

## Oral Sessions – Wednesday Afternoon

\*Signifies Presenting Author, when noted

### High Energy X-ray Microscopy

Lasalle B

Chair: **J. Almer**, APS - Argonne National Laboratory, Argonne, IL, USA, almer@anl.gov  
Co-Chair: **S. Stock**, Feinberg School of Medicine, Northwestern University, Chicago, IL, USA, s-stock@northwestern.edu

1:30	S-45	Invited - X-ray Diffraction Tomography of Polycrystalline Materials: Present and Future <b>S.R. Stock*</b> , Northwestern University, Chicago, IL, USA <b>J.D. Almer</b> , Argonne National Laboratory, Argonne, IL, USA <b>H. Birkedal</b> , Aarhus University, Aarhus, DK
2:00	D-48	Using Far Field High Energy Diffraction Microscopy to Characterize the State of Polycrystalline Material <b>J.-S. Park</b> , Argonne National Laboratory, Lemont, IL, US
2:20	D-60	Diffraction Scattering Computed Tomography: 3D Imaging of Complex Nanomaterials <b>M. E. Birkbak*</b> , <b>S. Frølich</b> , <b>S. Siddiqui</b> , <b>H. Birkedal</b> , Aarhus University, Aarhus, Denmark <b>J. D. Almer</b> , Argonne National Laboratory, Argonne, IL, USA <b>S. R. Stock</b> , Northwestern University, Chicago, IL, USA
2:40	S-31	Optimized Information Extraction from Near-field High Energy Diffraction Microscopy Data Sets <b>R. Suter</b> , <b>D. Mensasche</b> , <b>H. Liu</b> , Carnegie Mellon University, Pittsburgh, PA, USA
3:00		<b>Break</b>
3:30	S-48	Invited - Multi-scale and Multi-informative Imaging of Structural Materials <b>M. Kimura*</b> , <b>Y. Takeichi</b> , <b>Y. Niwa</b> , <b>H. Nitani</b> , High Energy Accelerator Res. Org. (KEK), Tsukuba, Ibaraki, Japan <b>M. Tomita</b> , <b>T. Inaguma</b> , <b>R. Murao</b> , Nippon Steel & Sumitomo Metal Co., Futtsu, Chiba, Japan <b>I. Obayashi</b> , <b>Y. Hiraoka</b> , Tohoku Univ., Sendai, Miyagi, Japan <b>Y. Liu</b> , Stanford Synchrotron Radiation Lightsource, Menlo Park, CA, USA <b>C. Holzner</b> , Carl Zeiss X-ray Microscopy, Pleasanton, CA, USA
4:00	D-55	3D Study of Deformation Behavior in Neutron Irradiated Fe 9Cr Alloy <b>X. Zhang*</b> , <b>J.S. Park</b> , <b>C. Xu</b> , <b>H. Sharma</b> , <b>J. Almer</b> , <b>M. Li</b> , Argonne National Laboratory, Lemont, IL, USA
4:20	D-96	High-energy X-ray Microscopy and Computed Tomography of Nuclear Fuels and Materials <b>M.A. Okuniewski*</b> , <b>F. Zhang</b> , <b>V. Ganapathy</b> , <b>P. Cassutt</b> , <b>B. Hamilton</b> , Purdue University, West Lafayette, IN, USA <b>H. Sharma</b> , <b>P. Kenesei</b> , <b>J. Almer</b> , Argonne National Laboratory, Argonne, IL, USA <b>J. Hunter</b> , <b>R. Pokharel</b> , <b>D. Brown</b> , Los Alamos National Laboratory, Los Alamos, NM, USA <b>A. Aitkaliyeva</b> , <b>J. Harp</b> , <b>B. Miller</b> , Idaho National Laboratory, Idaho Falls, ID, USA

### Trace Analysis

Lasalle C

Chair: **M.A. Zaitz**, IBM, Hopewell Junction, NY, USA, zaitz@us.ibm.com  
Co-Chair: **A. Martin**, Thermo Fisher Scientific, The Woodlands, TX, USA, al.martin@thermofisher.com

1:30	F-53	Invited - Analytical Options for Trace Analysis in WDXRF <b>A. Martin</b> , Thermo Scientific, West Palm Beach, FL, USA <b>A. McWilliams</b> , Research Triangle Institute, Durham, NC, USA
2:00	F-35	Micro-XRF Spectroscopy in Fossil Samples Providing Information about Preservation, Paleoecology and Evolution of Specimens <b>L. Maldanis*</b> , <b>D. Galante</b> , <b>C. A. Perez</b> , Brazilian Synchrotron Light Laboratory, Campinas, Brazil <b>J. Xavier-Neto</b> , Brazilian Biosciences National Laboratory, Campinas, Brazil <b>F. Rodrigues</b> , University of Sao Paulo, São Paulo, Brazil
2:20	S-47	Chemical Shift Measurements for Elemental Oxidation State Determination using a Cryogen-Free Microcalorimeter X-ray Spectrometer

**G. Havrilla\***, K. McIntosh, M. Croce, M. Rabin, S. Kosimor, Los Alamos National Laboratory, Los Alamos, NM, USA  
**R. Cantor, M. Carpenter, A. Hall**, Star Cryoelectronics, Santa Fe, NM, USA  
**D. Schmidt, D. Sweta, J. Ullom**, National Institute of Standards and Technology, Boulder, CO, USA  
**H. Naito**, H.K.N. Inc, San Jose, CA, USA

2:40	F-46	Discriminating Window and Bottle Glass Fragments Based on Trace Elements <b>B. Scruggs</b> , EDAX Inc., Mahwah, NJ, USA
3:00		<b>Break</b>
3:30	S-46	Invited - Outstanding and Environmentally-Friendly Tool for Trace Analysis: Benchtop TXRF <b>R. Ayala</b> , Fisichem Inc., Miami, FL, USA and Fisichem, Guatemala, Guatemala
4:00	F-3	An Energy-Dispersive XRF Analyser with X-ray Optics for Analysis of Heavy Elements in Water and Food at Parts-Per-Billion Concentrations <b>Y. Van Haarlem, E. Jager, P. Hodgins, J. Tickner</b> , CSIRO, Sydney, NSW, Australia
4:20	F-13	Optimization of X-ray Band-Pass-Filter to Analyze Traces in Organic or Inorganic Samples <b>J. Heckel</b> , SPECTRO Analytical Instruments GmbH, Kleve, Germany

### Biological Applications of X-ray Fluorescence Microscopy – Biomedical Applications

Lakeshore A

Chair:	<b>G. Woloschak</b> , Northwestern University, Feinberg School of Medicine, Chicago, IL, USA, g-woloschak@northwestern.edu	
1:30	B-26	Invited - The Role of Copper in Neurodegenerative Diseases <b>L.M. Miller</b> , Brookhaven National Laboratory, Upton, NY
2:00	B-21	Invited - Quantitative Subcellular Mapping of Metals Fluxes Reveals New Pathways in Microbial Physiology and Mammalian Development <b>T.V. O'Halloran*, A. Bayer, H. Chen, S. Garwin, A. Mendoza, A. Nowakowski, S. Wang, J. Deng, C. Jacobsen, N. Zhang, T.K. Wookruff</b> , Northwestern University, Evanston, IL, USA <b>S. Chen, S. Vogt</b> , APS, Argonne National Laboratory, Lemont, IL, USA
2:30	B-5	Permeability of Mammary Ductal Lumens to MRI Contrast Agents may be a New Marker for In Situ Mammary Cancer: An X-ray Fluorescence Microscopy Study <b>D. Mustafi*, E. Markiewicz, U. Dougherty, M. Zamora, J. Mueller, S.D. Conzen, G.S. Karczmar</b> , The University of Chicago, Chicago, IL, USA <b>S.-C. Gleber, S. Vogt</b> , APS, Argonne National Laboratory, Lemont, IL, USA
2:50	B-20	X-ray Fluorescence Imaging of Chemical Warfare in the Immune System Response: The Battle between Monocytes and Cryptococcus Neoformans <b>P.A. Lay, * R. Mak, J. Lee, P.-G. Juillard, T.C. Sorrell, G.E.R. Grau</b> , The University of Sydney, Sydney, Australia <b>S. Chen, J. Den, S. Vogt</b> , Argonne National Laboratory, Argonne, IL, USA
3:10		<b>Break</b>
3:40	B-19	Invited - XFM and XAS Combined Yield Insight on Mammalian Selenium Biochemistry <b>H. Harris, C. Weekley, M. Ceko, R. Rodgers</b> , The University of Adelaide, Adelaide, Australia <b>P. Witting</b> , The University of Sydney, Sydney, Australia
4:10	B-9	The Role of Storage Vesicles in Mammalian Copper Homeostasis <b>M. Ralle, T.R. Capps, M.E. Duffy</b> , Oregon Health and Sciences University, Portland, OR, USA <b>D. Vine, S. Vogt</b> , APS, Argonne National Laboratory, Argonne, IL, USA
4:30	B-18	Zinc Dynamics Regulate Germline Development in Caenorhabditis Elegans <b>A. Mendoza*, C. Schiffer, S. Cheung, S. Wignall, T.V. O'Halloran</b> , Northwestern University, Evanston, IL, USA <b>S. Vogt</b> , Argonne National Laboratory, Argonne, IL, USA
4:50	B-24	Investigation of Animal Tissue Samples using X-ray Fluorescence <b>T. Paunesku, A. Gordon, K. Harris, M.B. Wanzer, A. Larson, G. Woloschak</b> , Feinberg School of Medicine, Northwestern University, Chicago, IL, USA <b>O. Antipova, L. Li, S. Chen, S. Vogt</b> , APS, Argonne National Laboratory, Argonne IL, USA

## New Developments in XRD & XRF Instrumentation I

Lasalle A

Chairs: **T. Fawcett, T. Blanton**, International Centre for Diffraction Data, Newtown Square, PA, USA, fawcett@icdd.com; tblanton@icdd.com

1:30	D-50	Feasibility Study of "1 Minute" Reciprocal Space Mapping <b>M. Hawkridge*</b> , PANalytical, Westborough, MA, USA <b>L. Grieger, J. Woitok</b> , PANalytical, B.V., Almelo, The Netherlands
1:45	D-40	The STOE STADI P with Ag K $\alpha_1$ -Radiation – Highest Versatility for XRD and PDF <b>T. Hartmann</b> , Stoe & Cie GmbH, Darmstadt, Germany
2:00	D-98	Subfiles and Classifications in the Powder Diffraction File™ <b>S. Kabekkodu, S. Gates-Rector, A. Gindhart, T. Blanton, T. Fawcett</b> , ICDD, Newtown Square, PA, USA
2:15	D-89	A Powerful Update: HighScore(Plus) v.4.5 <b>T. Degen, E. Bron, M. Gateshki, M. Sadki</b> , PANalytical B.V., Almelo, Netherlands
2:30	D-37	Sample Temperature Accuracy of the Novel TTK 600 Low-Temperature Chamber <b>B. Puhr*, A. Pein</b> , Anton Paar GmbH, Graz, Austria
2:45	S-12	Novel, High Brightness X-ray Source and High Efficiency X-ray Optics for a New Generation of X-ray Instrumentation <b>W. Yun*, B. Stripe, J. Kirz, A. Lyon, D. Reynolds, S.J.Y. Lewis, S. Chen, V. Semenov, R.I. Spink, S.H. Lau</b> , Sigray, Concord, CA, USA
3:00	F-50	The Quantum Leap in ED-XRF - How Advanced Technologies Have Changed the Game <b>D. Sachtler, D. Wissmann</b> , SPECTRO Analytical Instruments GmbH, Kleve, Germany <b>M. Daniel-Prowse*</b> , SPECTRO Analytical Instruments Inc., Mahwah, NJ, USA
3:15		Break
3:45	D-45	Bright. Brighter. Unique - The New Incoatec Microfocus X-ray Source $\mu$ S 3.0 for Crystallography <b>B. Hasse, A. Stricker, J. Graf, A. Kleine, J. Wiesmann, C. Michaelsen</b> , Incoatec GmbH, Geesthacht, Germany
4:00	F-42	Newly Developed Compact Sized X-ray Sources <b>T. Parker, R. Steck, B. Harris, K. Kozaczek, C. Smith, E. Miller, S. Kamtekar</b> , Moxtek Inc., Orem, UT, USA
4:15	S-19	Analysis of Hermetically Closed Detector Modules for X-ray Detection <b>H. Soltau, A. Niculae*, H. Schmidt, R. Lackner, B. Talbi</b> , PNDetector GmbH, Munich, Germany
4:30	F-28	Hybrid Pixel Detector for XRF <b>E. Nygård, N. Malakhov</b> , Enxense AS, Asker, Norway <b>P. Weilhammer</b> , CERN, Geneva, Switzerland <b>K. Yamamoto, T. Nagano</b> , Hamamatsu Photonics, Hamamatsu City, Japan
4:45	D-39	PILATUS3 R CdTe Large-Area Detectors for Laboratory Applications <b>M. Mueller*, T. Donath, M. Rissi, C. Schulze-Briese</b> , DECTRIS Ltd, Baden, Switzerland
5:00	F-25	New Developments in the Field of Silicon Drift Detectors and Digital Signal Processing <b>A. Pahlke, R. Fojt, M. Fraczek, J. Knobloch, E. Lechner, N. Miyakawa, J. Rumpff, O. Scheid, A. Simsek, C. Zacher</b> , KETEK GmbH, Munich, Germany

## X-ray Imaging I

Madison

Co-Chairs: **M. Behr**, The Dow Chemical Company – MIOPS, Midland, MI, USA, mjbehr@dow.com

**M. Denecke**, Dalton Nuclear Institute, The University of Manchester, Manchester, United Kingdom, melissa.denecke@manchester.ac.uk

**G. Havrilla**, Los Alamos National Laboratory, Los Alamos, NM, USA, havrilla@lanl.gov

1:30	S60	Invited - High Resolution Microscopy with Coherent X-rays <b>C. Schroer</b> , DESY/PETRAIII, Hamburg, Germany
2:00	S-29	Use of Energy Scanned Beams for Coherent X-ray Diffraction Imaging <b>W. Cha, S. Hruszkewycz, A. Ulvestad, R. Sichel-Tissot, M. J. Highland, P. H. Fuoss, R. Harder, W. Liu, J. Maser</b> , Argonne National Laboratory, Argonne, IL, USA <b>M. Allain, V. Chamard</b> , Aix-Marseille University, CNRS, Marseille, France

2:20	<b>D-70</b>	Applications of Full Field X-ray Diffraction Microscopy in the Heteroepitaxial Thin Film Materials <b>Z. Zhang*</b> , <b>S. Chang</b> , <b>J.W. Freeland</b> , <b>H. Liu</b> , <b>H. Zhou</b> , <b>D. Fong</b> , Argonne National Laboratory, Argonne, IL, USA <b>N. Laanait</b> , Oak Ridge National Laboratory, Oak Ridge, TN, USA
2:40	<b>S-25</b>	Imaging Lateral Inhomogeneity in Ingan Heterostructures with X-ray Microdiffraction <b>R. Sichel-Tissot*</b> , <b>S.O. Hruskewycz</b> , <b>M.V. Holt</b> , <b>W. Cha</b> , <b>M. Highland</b> , <b>E. Karapetrova</b> , <b>P.H. Fuoss</b> , Argonne National Laboratory, Argonne, IL, USA <b>S.R. Lee</b> , <b>D.D. Koleske</b> , Sandia National Laboratories, Albuquerque, NM, USA
3:00		<b>Break</b>
3:30	<b>D-59</b>	Invited - X-ray Physicochemical Imaging of Working Catalysts <b>A.M. Beale*</b> <b>A. Vamvakeros</b> , <b>P. Senecal</b> , UCL, London, UK <b>S.D.M. Jacques</b> , UoM, Manchester, UK <b>M. Di Michiel</b> , ESRF, Grenoble, France <b>J.F.W. Mosselmans</b> , <b>S.W.T. Price</b> , Diamond Light Source, Didcot, UK
4:00	<b>D-19</b>	Operando Microdiffraction Mapping of Single Particle Cathode Materials <b>B.M. May*</b> , <b>J. Cabana</b> , University of Illinois at Chicago, Chicago, IL, USA <b>K. Wiaderek</b> , <b>O. Borkiewicz</b> , <b>R. Xu</b> , <b>P. Chupas</b> , <b>K. Chapman</b> , APS, Argonne National Laboratory, Argonne, IL, USA <b>N. Faenza</b> , <b>N. Pereira</b> , <b>G.G. Amatucci</b> , Rutgers University, North Brunswick, NJ, USA
4:20	<b>S-3</b>	Progress of Analytical Imaging with High-energy X-ray Compton Scattering <b>Y. Sakurai*</b> , <b>M. Itou</b> , <b>M. Brancewicz</b> , Japan Synchrotron Radiation Research Institute, Sayo, Hyogo, Japan <b>H. Sakurai</b> , <b>K. Suzuki</b> , Gunma University, Kiryu, Gunma, Japan <b>B. Berbiellini</b> , <b>A. Bansil</b> , Northeastern University, Boston, MA, USA <b>Y. Orikasa</b> , <b>Y. Uchimoto</b> , Kyoto University, Kyoto, Japan
4:40	<b>S-21</b>	Advances in X-ray Diffraction Computed Tomography: Removing Single Crystal Artefacts and Bridging the Gap Between Spatial and Temporal Resolution <b>A. Vamvakeros</b> , <b>A.M. Beale</b> , University College London & Research Complex at Harwell, London, UK <b>S.D.M. Jacques</b> , University of Manchester, Manchester, UK and University College London & Research Complex at Harwell, London, UK <b>M. Di Michiel</b> , ESRF, Grenoble, France <b>V. Middelkoop</b> , Flemish Institute for Technological Research (VITO), Mol, Belgium

## Oral Sessions – Thursday Morning

\*Signifies Presenting Author, when noted

### Rietveld

### Lasalle B

Chair: **S. Lapidus**, APS - Argonne National Laboratory, Argonne, IL, USA, [slapidus@aps.anl.gov](mailto:slapidus@aps.anl.gov)

- 8:30 D-67 Invited - Unraveling Structural Details in Negative Thermal Expansion Materials  
**C. Lind-Kovacs\***, **T.I. Baiz**, **A. Gindhart**, **J. Gradient**, **L. Lovings**, **L. Young**, The University of Toledo, Toledo, OH, USA  
**J.S. O. Evans**, Durham University, Durham, UK
- 9:00 D-2 Nitrogen Doping: A Universal Method to Tune the Electronic Structure and Enhance Luminescent Performance of Intrinsic Scintillator  
**G.M. Cai**, **Z.X. Wang**, **Z.P. Jin**, Central South University, Changsha, Hunan, China
- 9:20 D-32 In Situ Crystallographic Thermal Expansion Measurements of Compounds in the  $\text{HfO}_2\text{-Ta}_2\text{O}_5\text{-TiO}_2$  Ternary System Using CTEAS  
**S.J. McCormack\***, **K.C. Seymour**, **W.M. Kriven**, University of Illinois at Urbana-Champaign, Champaign, IL, USA
- 9:40 D-74 Invited - Structure Solution from Powder Data Using a Symmetry-Mode Parameter Set  
**B.J. Campbell**, Brigham Young University, Provo, Utah, USA
- 10:10 Break
- 10:40 D-34 Invited - Manifestation of Itinerant Magnetism in Hole-Doped Iron Arsenide Superconductors  
**J.M. Allred\***, University of Alabama, Tuscaloosa, AL, USA  
**K.M. Taddei**, **M.J. Krogstad**, **D.E. Brown**, **O. Chmaissem**, Northern Illinois University, De Kalb, IL, USA  
**D.E. Bugaris**, **S.H. Lapidus**, **D.Y. Chung**, **H. Claus**, **M.G. Kanatzidis**, **S. Rosenkranz**, **R. Osborn**, Argonne National Lab, Lemont, USA  
**J. Kang and R.M. Fernandes**, University of Minnesota, Minneapolis, MN, USA  
**I. Eremin**, Ruhr-Universität Bochum, Bochum, Germany
- 11:10 D-33 Subsolidus Phase Relations and Crystal Structures of New Compounds in  $\text{Li}_2\text{O}/\text{WO}_3\text{-In}_2\text{O}_3\text{-TiO}_2$  Ternary Systems  
**L.M. Su**, **G.M. Cai\***, **X. Fan**, **Z.P. Jin\***, Central South University, Changsha, Hunan, China
- 11:30 D-52 Effect of Fluorescence on Quantitative X-ray Diffraction Estimates of Crystalline and Amorphous Phases in Fe-Rich Geologic Samples Using Co And Cu Radiations  
**N.M. Piatak\***, **C.J. Green**, U.S. Geological Survey, Reston, VA, USA
- 11:50 D-90 Rietveld Amorphous Quantification, Now Even More Painless  
**A. Adibhatla**, PANalytical Inc., Westborough, USA  
**T. Degen**, **U. König**, **N. Norberg**, PANalytical B.V., Almelo, Netherlands

### Industrial Applications of XRF

### Lasalle C

Chair: **D. Broton**, Construction Technology Labs, Skokie, IL, USA, [dbroton@ctlgroup.com](mailto:dbroton@ctlgroup.com)

- 9:00 S-54 Invited - X-rays in Cement Production  
**E. Watson**, Holcim (US) Inc., Bloomsdale, MO, USA
- 9:30 F-48 Re-Melting Tin-Bismuth and Tin-Indium Solder Samples for XRF Analysis in Order to Eliminate Microstructural Effects  
**T. Gorewoda**, **J. Anyszkiewicz**, **Z. Mzyk**, **S. Malara**, **K. Bilewska**, **A. Cybulski**, **J. Golebiowska – Kurzawska**, **M. Knapik**, **M. Grzegorczyk** and **J. Kostrzewska**, Institute of Non-Ferrous Metals, Gliwice, Poland
- 9:50 F-49 The Development of a New Sample Preparation Procedure for the Analysis of CuAgP Solder by XRF Spectrometry  
**J. Anyszkiewicz**, **T. Gorewoda**, **Z. Mzyk**, **S. Malara**, **K. Bilewska**, **A. Cybulski**, **J. Golebiowska-Kurzawska**, **M. Knapik**, **M. Grzegorczyk**, **J. Kostrzewska**, Institute of Non-Ferrous Metals, Gliwice, Poland

<b>10:10</b>	<b>F-16</b>	Coating Thickness by XRF – How to Decide if Microspot, Benchtop or Handheld Instrumentation is Right for You <b>M. Kreiner</b> , Oxford Instruments, Concord, MA, USA
<b>10:30</b>		<b>Break</b>
<b>10:50</b>	<b>F-51</b>	Analysis of Light Elements by Benchtop EDXRF <b>D. Pecard*</b> , <b>K. Odegaard</b> , <b>A. Buman</b> , Bruker AXS, Madison, WI, USA
<b>11:10</b>	<b>F-38</b>	Nutrients in Biomass – Benefits of Using WD-XRF <b>J. Sedlmair</b> , Bruker AXS Inc., Madison, WI, USA <b>A. Roa-Espinosa</b> , Soil Net LLC, Madison, WI, USA <b>T. Vu</b> , University Wisconsin-Madison, Madison, WI, USA
<b>11:30</b>	<b>F-30</b>	DANTE, A Compact and Low-Power Digital Pulse Processor to Exploit CUBE Preamplifier Ultimate Energy Resolution and High-Count Rate Capability <b>L. Bombelli*</b> , <b>M. Manotti</b> , <b>R. Alberti</b> , <b>T. Frizzi</b> , XGLab SRL, Milano, Italy
<b>11:50</b>	<b>F-55</b>	SDD X-ray Spectrometer with Improved High Energy Response and Counting Rate Performance <b>Y. Wang</b> , <b>S. Barkan</b> , <b>V.D. Saveliev</b> , <b>L. Feng</b> , <b>M. Zhang</b> , <b>B. Goolsby</b> , <b>Y. Tomimatsu</b> , <b>E.V. Damron</b> , Hitachi High-Technologies Science America, Inc., Northridge, USA
<b>12:10</b>	<b>F-15</b>	Electronically Fused Beads & the Reliable Measurement of F, S and Cl in Cement <b>B. Werner</b> , Apex Marketing, Brighton, MI, United States <b>R. Schramm</b> , Fluxana GmbH, Bedburg-Hau, Germany

#### Biological Applications of X-ray Fluorescence Microscopy –Plant/Environmental/Microbial Science Lakeshore A

---

Chair: **T. Lanzirotti**, GSECARS, The University of Chicago and Argonne National Laboratory, Chicago, IL, USA, [lanzirotti@uchicago.edu](mailto:lanzirotti@uchicago.edu)

<b>8:30</b>	<b>B-25</b>	Invited - Synchrotron Based Exploration of Aerosol Phosphorus and Iron Composition: Implications for Ocean Productivity <b>E. Ingall</b> , Georgia Institute of Technology, Atlanta, GA, USA
<b>9:00</b>	<b>B-22</b>	Invited - Plant and Soil Sciences Research Cultivated by X-ray Fluorescence Microscopy <b>R. Tappero</b> , Brookhaven National Laboratory, Upton, NY, USA
<b>9:30</b>	<b>B-23</b>	Invited - Marriage of X-ray Spectroscopy and Microscopy for Trace Element Analysis in Environmental and Biological Systems <b>B. Mishra</b> , Illinois Institute of Technology, Chicago, IL, USA and Argonne National Laboratory, Lemont, IL, USA
<b>10:00</b>		<b>Break</b>
<b>10:30</b>	<b>B-4</b>	X-ray Fluorescence Tomographic Imaging of Bacteria within Soil Aggregates <b>K.M. Kemner*</b> , <b>S.L. O'Brien</b> , <b>D. Sholto Douglas</b> , <b>D. Gursory</b> , <b>B. Lai</b> , <b>C. Roehrig</b> , <b>S. Sullivan</b> , <b>S. Vogt</b> , Argonne National Laboratory, Argonne, IL, USA <b>M.D. Whiteside</b> , <b>Vrije Universiteit</b> , Amsterdam, Holland <b>A. Dohnalkova</b> , <b>L. Kovarik</b> , Pacific Northwest National Laboratory, Richland, Washington, USA <b>D.M. Durall</b> , <b>M.D. Jones</b> , University of British Columbia, Okanagan, Canada
<b>10:50</b>	<b>B-6</b>	K And Ca in Leaves of Arabidopsis Thaliana: An Approach Using Total Reflection X-ray Fluorescence and Micro X-ray Fluorescence <b>U. Fittschen</b> , <b>R. Hoehener</b> , <b>S. Tabatabaei</b> , <b>H.-H. Kunz</b> , Washington State University, Pullman, WA, USA <b>M. Radtke</b> , BAM – Federal Institute for Materials Research and Testing, Berlin, Germany
<b>11:10</b>	<b>B-8</b>	Evaluation of Ti Levels in Water Samples Exposed to Different Concentrations of TiO <sub>2</sub> Nanoparticles by Portable XRF and TXRF <b>T. Galvão</b> , <b>C. Appoloni</b> , State University of Londrina - UEL, Londrina, PR, Brazil <b>T. do Carmo</b> , <b>M. Fernandes</b> , Federal University of São Carlos, São Carlos, SP, Brazil
<b>11:30</b>	<b>B-13</b>	X-ray Fluorescence Microscopy as a Tool to Study the Effects of Moisture on Ion Transport in Wood Cell Walls <b>J.E. Jakes*</b> , <b>S.L. Zelinka</b> , <b>C.G. Hunt</b> , <b>C.R. Frihart</b> , <b>D.J. Yelle</b> , <b>L. Lorenz</b> , <b>G.T. Kirker</b> , USDA Forest Service, Forest Products Laboratory, Madison, WI, USA <b>S. Vogt</b> , <b>D. Vine</b> , <b>S.C. Gleber</b> , <b>S. Chen</b> , Argonne National Laboratory, Argonne, IL, USA

## New Developments in XRD & XRF Instrumentation II

Lasalle A

Chairs: **T. Fawcett, T. Blanton**, International Centre for Diffraction Data, Newtown Square, PA, USA, fawcett@icdd.com;tblanton@icdd.com

8:30	D-91	Certification of SRM 1979; Line Profile Standard for Analysis of Crystallite Size <b>J.P. Cline, M.H. Mendenhall, J.J. Ritter, D. Black, A. Henins, J.E. Bonevich</b> , NIST, Gaithersburg, MD, USA <b>P. Whitfield</b> , Oak Ridge National Laboratory, Oak Ridge, TN, USA
8:50	S-26	ADIS, A New X-ray Diffraction & X-ray Fluorescence System for In Situ Material Characterization for Cultural Heritage <b>V. Aguilar*, J.L. Ruvalcaba, L. Bucio</b> , Instituto de Fisica, Universidad Nacional Autonoma de Mexico, Mexico City, Mexico
9:10	D-20	New Neutron Time-of-Flight (TOF) Capability in PDF-4+ Relational Databases: Digitized Diffraction Patterns and I/Ic for Quantitative Phase Analysis <b>J. Faber</b> , Faber Consulting, Thornton, PA, USA <b>S. Kabekkodu, J. Blanton, T. Blanton, T. Fawcett</b> , ICDD, Newtown Square, PA, USA
9:30	D-99	Enhanced Ab Initio Indexing of TOF Neutron Powder Diffraction Data using Maximum Entropy <b>R.J. Papoulier</b> , IRAMIS / LLB / CEA-Saclay, Gif-sur-Yvette, France <b>T.N. Blanton, J.R. Blanton, S.N. Kabekkodu</b> , ICDD, Newtown Square, PA, USA <b>J.G. Faber</b> , Faber Consulting, Inc., Thornton, PA, USA
9:50	D-21	The Commission of Powder X-ray Diffraction at Taiwan Photon Source <b>H.-S. Sheu,* Y.-C. Chuang, C.-K. Chang, Y.-C. Lai, K.-L. Yu, L. Lee</b> , National Synchrotron Radiation Research Center, Hsinchu, Taiwan
10:10		<b>Break</b>
10:40	S-30	Advances and Future Directions in 3D X-ray Microscopy: Orientation and <i>k</i> -space <b>J.Z. Tischler, W. Liu, R. Xu</b> , Argonne National Lab, Argonne IL, USA
11:00	D-15	Phase-Specific XRD <b>G. Hansford</b> , University of Leicester, Leicester, UK
11:20	S-6	First Indirect X-ray Imaging Tests with an 88-mm Diameter Single Crystal <b>A. Lumpkin</b> , FNAL, Batavia, IL, USA <b>A. Macrander</b> , ANL, Argonne, IL, USA
11:40	S-50	Three Crystals Spectrometer for High Energy Resolution Fluorescence Detected X-ray Absorption Spectroscopy and X-ray Emission Spectroscopy at SSRF <b>P. Duan, J. Li, S. Gu, H. Cao, X. Wei, Y. Huang*</b> , Shanghai Synchrotron Radiation Facility, Chinese Academy of Sciences, Shanghai, China

## Cultural Heritage

Madison

Chair: **R. van Grieken**, University of Antwerp, Antwerp, Belgium, rene.vangrieken@uantwerpen.be

8:30	S-2	Invited - Synergy of Nuclear, Atomic and Molecular Methodologies Applied to the Study of Cultural Heritage - The Prominent Role of XRF <b>C. Appoloni</b> , State University of Londrina - UEL, Londrina, PR, Brazil
9:00	D-82	Characterization Techniques Used in the Forensic Analysis of a Metal Art Object <b>K. Cunningham*, C. Carta, M. Flores, M. Goorsky, I. Kakoulli</b> , University of California, Los Angeles, Los Angeles, CA, USA
9:20	S-39	Depth Profiling of Artists' Acrylic Paint Films with X-ray Absorption Spectroscopy <b>E.A. Willneff*, S.L.M. Schroeder</b> , University of Leeds, Leeds, UK <b>B.A. Ormsby</b> , Tate, London, UK
9:40	F-32	Visualizing and Analysis of $\mu$ XRF Scanning Images in Arts and Conservation <b>M. Buegler, R. Tagle, F. Reinhardt</b> , Bruker Nano GmbH, Berlin, Berlin, Germany
10:00		<b>Break</b>

- 10:30**      **S-28**      Invited - Portable EDXRF for Cultural Heritage: The Need of a Multidisciplinary Approach  
**S. Ridolfi**, Ars Mensurae, Rome, Italy
- 11:00**      **S-27**      Non-Destructive XAS Analysis of Pigments Using High-Throughput Gas-Flow Total Electron-Yield Detection  
**S. Schroeder, E. Willneff**, University of Leeds, Leeds, UK  
**J. Thomas**, University of Goteborg, Goteborg, Sweden  
**N. Eastaugh**, Art Analysis & Research, London, UK  
**N. Tsapatsaris**, European Spallation Source, Lund, Sweden
- 11:20**      **F-4**      A Novel Mobile MA-XRF Scanner for a (Near) Real-Time Elemental Imaging of Painted Artworks  
**F. Paolo Romano**, IBAM-CNR, Catania, Italy  
**C. Caliri, H.C. Santos**, INFN-LNS, Catania, Italy  
**S. Di Martino, P. Nicotra**, SIATEL, Catania, Italy  
**F. Rizzo**, University of Catania, Catania, Italy
- 11:40**      **F-29**      "Crono": a Reconfigurable MACRO-XRF Scanner for Cultural Heritage Applications  
**R. Alberti, T. Frizzi\***, L. Bombelli, M. Gironda, N. Aresi, XGLab SRL, Milano, Italy  
**C. Miliani, F. Rosi, L. Cartechini**, CNR-ISTM, Perugia, Italy
- 12:00**      **S-7**      Simultaneous X-ray Diffraction and Fluorescence with the pnCCD: A New Technique for Cultural Heritage Science  
**J. Davis\*, J. Schmidt, M. Huth, S. Ihle, D. Steigenhöfer, Heike Soltau**, PNDetector, München, Bayern, Deutschland  
**R. Hartman, P. Holl, G. Lutz, L. Strüder**, PNSensor, München, Bayern, Deutschland

## Oral Sessions – Thursday Afternoon

\*Signifies Presenting Author, when noted

### Applied Materials I

Lasalle B

Chairs: **T. Fawcett, T. Blanton**, ICDD, Newtown Square, PA, fawcett@icdd.com; tblanton@icdd.com

- 1:30 D-71 Invited - X-ray Diffraction Investigations in the Smithsonian Gem and Mineral Collection  
**J. Post**, Smithsonian Institution, Washington, DC, USA
- 2:00 D-7 Phase Relations of Anhydrous and Hydrous Earth Alkali Aluminates with Calcium, Strontium and Barium Solid Solution of Binary Ca-Ba-, Ca-Sr- and Ba-Sr –Aluminates and Their Hydrates  
**H. Poellmann, R. Kaden**, University of Halle, Halle, Germany
- 2:20 D-3 Synthesis and Structural Characterization of Oxsilicate Apatite  $\text{Ln}_8\text{Sr}_2(\text{SiO}_4)_6\text{O}_2$   
**J.X. Wang, Z. L. Dong\***, Nanyang Technological University, Singapore, Singapore
- 2:40 D-44 X-ray Diffraction Analysis of the Defect Structure of Freestanding Diamond Substrates and Homoepitaxial Diamond Films  
**L. Kirste, V. Zürbig, C. Schreyvogel, C.J. Widmann, B. Tegetmeyer, M. Prescher, V. Cimalla, C.E. Nebel**, Fraunhofer Institute for Applied Solid State Physics (IAF), Freiburg, Germany
- 3:00 Break
- 3:30 D-93 Invited - X-ray Total Scattering Analysis Electrochemically Active  $\text{MnO}_2$  Nanosheet Assemblies  
**S. Misture, P. Metz, P. Gao**, Alfred University, Alfred, NY, USA
- 4:00 D-17 Rational Design of Catalysts Using In Situ PXRD as a Tool for Understanding Catalytic Deactivation  
**D.H. Barrett, C.B. Rodella**, Brazilian Synchrotron Light Laboratory (LNLS)/Brazilian Center for Energy and Materials Research (CNPEM), Campinas, Brazil  
**M.S. Scurrell**, University of South Africa, Johannesburg, South Africa  
**B. Diaz**, Canadian Light Source, Saskatoon, Canada  
**P.J. Franklyn**, University of the Witwatersrand, Johannesburg, South Africa
- 4:20 D-84 In Situ High-Energy X-ray Study of Synthesis and Transformation of Applied Materials  
**Y. Ren**, Argonne National Laboratory, Argonne, IL, USA
- 4:40 S-40 In Situ EXAFS Study of Metallic Tin/Graphite Composite Anodes for Lithium-Ion Batteries  
**Y. Ding\*, C. Segre**, Illinois Institute of Technology, Chicago, IL, USA
- 5:00 D-9 Structural Design and Characterization of Vanadium-Based Phosphates as Cathode Materials for Li-Ion Batteries  
**Q. Kuang\*, Y.M. Zhao**, South China University of Technology, Guangzhou, China

### General XRD

Lasalle C

Chair: **C. Murray**, IBM T.J. Watson Research Center, Yorktown Heights, NY, conal@us.ibm.com

- 1:40 D-66 X-ray Diffraction Study on AlGaAs/AlAs Distributed Bragg Reflector  
**C. Li\***, **M.S. Goorsky**, University of California, Los Angeles, Los Angeles, CA, USA
- 2:00 D-65 Study on Atomic-Layer-Deposited  $\text{Al}_2\text{O}_3$  Dielectric Films with a New Small Angle X-ray Scattering (SAXS) Method  
**C. Li\***, **F. Shahriarian, M.S. Goorsky**, University of California, Los Angeles, Los Angeles, CA, USA
- 2:20 D-27 Mapping of Spatial Inhomogeneities with Laboratory X-ray Diffraction  
**M. Wolf\***, **S. Khawaja, J. Cabana**, University of Illinois Chicago, Chicago, IL, USA
- 2:40 S-32 Side-coated TAGwoods and the Formation of Dense Aggregates of Intertwined TAGwood Snakes  
**F. Peyronel, A. Marangoni**, University of Guelph, Guelph, Ontario, Canada  
**B. Quinn, D. Pink**, St. Francis Xavier University, Antigonish, Nova Scotia, Canada

3:00		<b>Break</b>
3:30	<b>D-103</b>	A Rigorous Analysis of the Scherrer Equation <b>S.-Y. Lee, I.C. Noyan</b> , Columbia University, New York, NY, USA
3:50	<b>D-85</b>	Improved Diffraction Analysis of Mesoporous Materials Using an Evacuated Beampath <b>S.A. Speakman</b> , PANalytical, Westborough, MA, USA <b>L. Bromberg</b> , MIT, Cambridge, MA, USA
4:10	<b>D-30</b>	A New Method for the Quantitative Phase Analysis Using Integrated Intensities and Chemical Compositions of Individual Crystalline Phases <b>H. Toraya</b> , Rigaku Corporation, Akishima, Tokyo, Japan
4:30	<b>D-73</b>	X-ray Diffraction Reveals Structural Aspects of Protein Assemblies in Connective Tissues <b>O. Antipova*</b> , XSD, Argonne National Laboratory, Lemont, IL, USA <b>T. Irving</b> , BioCAT, Illinois Institute of Technology, Chicago, IL, USA <b>B. Sullivan</b> , Purdue University, West Lafayette, IN, USA
4:50	<b>D-104</b>	The Relation between Sampling and Intensity Statistics of Diffraction from Nanocrystalline Powders <b>H. Öztürk, I.C. Noyan</b> , Columbia University, New York, NY, USA <b>H. Yan, J.P. Hill</b> , NSLS, Brookhaven National Laboratory, Upton, NY, USA

## General XRF

## Lasalle A

Chair: **M. Schmeling**, Loyola University Chicago, Chicago, IL, USA, mschmel@luc.edu

2:00		Invited - Particle Induced X-ray Screening of Consumer Products for Flame Retardants <b>G. Peaslee</b> , Hope College, Holland, MI, USA
2:30	<b>F-43</b>	Invited - XRS of Atmospheric Aerosols for Preventive Conservation and Climate Change Research <b>R. Van Grieken</b> , University of Antwerp, Antwerp, Belgium
3:00	<b>F-45</b>	New Developments in Real-Time Processing and Display of Spectra from a Multipixel Microcal X-ray Detector <b>T. Jach*</b> , NIST, Gaithersburg, MD, USA <b>S. Thurgate</b> , Murdoch University, Perth, WA, Australia <b>R. Cantor</b> , Star Cryoelectronics, Santa Fe, NM, USA <b>J. Ullom</b> , NIST, Boulder, CO, USA
3:20	<b>F-61</b>	Compact Scanning Device with Variable Spot Size in the mm Range for Large Area Macro-Scans <b>P. Wobrauschek, P. Allinger, A. Utz, S. Smolek, D. Ingerle, TU Wien</b> , Atominstitut, Vienna, Austria
3:40		<b>Break</b>
4:00	<b>F-34</b>	Invited - Using Energy Dispersive X-ray Fluorescence to Determine Trace and Toxic Elements in Human Tissues, In Vivo and Ex Vivo <b>A. Pejovic-Milic, E. Da Silva</b> , Ryerson University, Toronto, ON, Canada
4:30	<b>F-33</b>	The Development of a Tomographic X-ray Fluorescence Microscopy at the 2-ID-E Beamline <b>L. Li, O. Antipova, S. Chen, D. Gursoy, S. Vogt</b> , Argonne National Laboratory, Lemont, IL, USA
4:50	<b>S-38</b>	In situ XAS Study of Structural Changes and Degradation Mechanisms in Li Rich Cathode Materials <b>S. Aryal, E. Temofeeva, C. Segre</b> , Illinois Institute of Technology, Chicago, IL, USA
5:10	<b>S-5</b>	XAES Observation of Nucleation Mechanism in Deposition of WS <sub>2</sub> <b>H. Zhang, A. Hock</b> , Illinois Institute of Technology, Chicago, IL, USA

Chair: **S. Vogt**, APS, Argonne National Laboratory, Argonne, IL, USA, svogt@aps.anl.gov

<b>1:30</b>	<b>B-14</b>	Invited - High-Resolution Trace Element Studies of Biological Tissues and Cells Using the Bionanoprobe at the Advanced Photon Source <b>S. Chen, S. Vogt, C. Jacobsen</b> , APS, Argonne National Laboratory, Argonne, IL, USA <b>T. Paunesku, G. Woloschak</b> , Feinberg School of Medicine, Northwestern University, Chicago, IL, USA <b>Q. Jin, Y. Hong, J. Deng</b> , Northwestern University, Evanston, IL, USA <b>K. Brister</b> , Northwestern Synchrotron Research Center, Northwestern University, Argonne, IL, USA
<b>2:00</b>	<b>B-7</b>	Invited - Illuminating the Redistribution Dynamics of Trace Metals During Cell Proliferation and Embryonic Development <b>C.J. Fahrni</b> , Georgia Institute of Technology, Atlanta, GA
<b>2:30</b>	<b>B-15</b>	APS 2-ID-D X-ray Fluorescence Microprobe: Instrumentation Advances <b>B. Lai*, C. Roehrig, S. Chen, Z. Cai, M. Wojcik, D. Shu, S. Gleber, S. Vogt</b> , APS, Argonne National Laboratory, Argonne, IL, USA
<b>2:50</b>		<b>Break</b>
<b>3:30</b>	<b>B-17</b>	Invited - Applications of X-ray Tomography Across Multiple Length Scales <b>P. Pianetta</b> , Stanford University, Menlo Park, CA, USA
<b>4:00</b>	<b>F-54</b>	Evaluation of Contemporary Data Acquisition Schemes for X-ray Fluorescence Tomography <b>D. Gursoy*</b> , <b>S. Sullivan, S. Vogt</b> , Argonne National Laboratory, Lemont, IL, USA
<b>4:20</b>	<b>B-16</b>	Breakthrough Developments in Laboratory MicroXRF to Enable Trace-Level Mapping and Femtogram Detection Sensitivity in Biological Specimens <b>B. Stripe, W. Yun, A. Lyon, D. Reynolds, S.J.Y. Lewis, S. Chen, V. Semenov, R.I. Spink, S.H. Lau</b> , Sigray, Concord, CA, USA

**X-ray Imaging II****Madison**

Co-Chairs: **M. Behr**, The Dow Chemical Company – MIOPS, Midland, MI, USA, mjbehr@dow.com

**M. Denecke**, Dalton Nuclear Institute, The University of Manchester, Manchester, United Kingdom, melissa.denecke@manchester.ac.uk

**G. Havrilla**, Los Alamos National Laboratory, Los Alamos, NM, USA, havrilla@lanl.gov

<b>1:30</b>	<b>S-55</b>	Invited - Spectroscopic X-ray Imaging for Studying Alterations at and Below the Surface of Fine Art Paintings, Stained Glass Windows and Illuminated Manuscripts <b>K. Janssens*</b> , <b>F. Vanmeert, G. Van der Snickt, S. Legrand</b> , University of Antwerp, Antwerp, Belgium
<b>2:00</b>	<b>S-34</b>	Soft X-ray Imaging of Modern and Contemporary Artists' Materials <b>E.A. Willneff*</b> , <b>S.L.M. Schroeder</b> , University of Leeds, Leeds, UK <b>B.A. Ormsby</b> , Tate, London, UK
<b>2:20</b>	<b>S-10</b>	Comparison of Wavelength-Dispersive and Energy-Dispersive XRF Imaging Methods <b>K. Tsuji*</b> , <b>Y. Takimoto, M. Yamanashi</b> , Osaka City University, Osaka, Japan <b>S. Kato, T. Yamada, T. Shoji, N. Kawahara</b> , Rigaku Co., Osaka, Japan
<b>2:40</b>	<b>F-52</b>	Increased XFI Fitting Turn-Over Rates via Abridged Spectral Matrix Inversion <b>A. Crawford, O. Ponomarenko, C. Simoens, G. George, I. Pickering</b> , University of Saskatchewan, Saskatoon, SK, Canada
<b>3:00</b>		<b>Break</b>
<b>3:30</b>		Invited - Title to be announced <b>M. Newville</b> , GSECARS, University of Chicago, Chicago, IL, USA
<b>4:00</b>	<b>S-4</b>	Pore Network Analysis of Carbonate Rocks by Tomographic Images Taken at Multiple Spatial Resolutions <b>R. Nagata, C. Appoloni</b> , State University of Londrina - UEL, Londrina, PR, Brazil <b>P. dos Reis</b> , Midwestern State University, Guarapuava, PR, Brazil
<b>4:20</b>	<b>S-9</b>	Quantitative Analysis of Calcium Oxide in Desiccant and Human Body <b>H. Tanioka</b> , Tanioka Clinic, Tokyo, Japan <b>K. Kaga</b> , National Institute of Sensory Organs, Tokyo, Japan

- 4:40**      **S-18**      Alloy Solidification Under External Fields via Time-Resolved Synchrotron Tomographic Quantification  
**P. Lee**, University of Manchester, Manchester, UK
- 5:00**      **F-68**      In situ Loading of Hyper Elastic Materials during Synchrotron 3D Tomographic Imaging  
**B. Patterson, K. Henderson, R. Pacheco, N.L. Cordes, J.C.E. Mertens**, Los Alamos National Laboratory, Los Alamos, NM, USA  
**N. Chawla, S. Singh, A.R. Ovehero, J. Williams**, Arizona State University, Tempe, AZ, USA  
**X. Xiao**, Argonne National Laboratory, Argonne, IL, USA

## Oral Sessions – Friday Morning

\*Signifies Presenting Author, when noted

### Stress Analysis

Lasalle A

Chair: **T.R. Watkins**, Oak Ridge National Laboratory, Oak Ridge, TN, watkinstr@ornl.gov

- 8:30 D-62 Invited - New Multi-axial Straining Devices for Neutron Diffraction  
**T. Gnäupel-Herold\***, **J. Milner**, NIST Center for Neutron Research, Gaithersburg, MD, USA
- 9:00 D-61 Internal Stresses and High Temperature Plasticity of a Single Crystal Superalloy: Real Time In Situ Experiments with Synchrotron X-ray Diffraction  
**T. Schenk**, **R. Trehorel**, **A. Jacques**, CNRS – Université de Lorraine, Nancy, France  
**J.B. Le Graverend**, Texas A&M University, Texas, TX, USA  
**J. Cormier**, CNRS-ENSMA-Université de Poitiers, Poitiers, France
- 9:20 D-68 Characterization of Residual Stress in Polycrystalline Diamond Composites Using Energy Dispersive Diffraction  
**J. Okasinski\***, **J.-S. Park**, APS, Argonne National Laboratory, Argonne, IL, USA  
**R.K. Viswanadham**, **S. Alkhalaileh**, IDS Group, Houston, TX, USA
- 9:40 D-25 Calculation of XRD Spectra of N-H Extended Solids Under High Pressure  
**I.G. Batyrev\***, **S.P. Coleman**, **J.P. Larentzos**, US Army Research Laboratory, Aberdeen Proving Ground, MD, USA
- 10:00 Break
- 10:20 D-10 Through Thickness Texture Gradient Prediction of 5XXX Series Aluminum After Sheet Rolling Operations  
**J. Ho\***, **S. Dennis**, Novelis, Inc., Kennesaw, GA, USA  
**H. Garmestani**, Georgia Institute of Technology, Atlanta, GA, USA
- 10:40 S-8 Coherent X-ray Imaging of 3D Dislocation Networks in Battery and Palladium Nanoparticles  
**A. Ulvestad**, **B. Stephenson**, Argonne National Laboratory, Lemont, IL, USA
- 11:00 D-14 Fundamental Understanding of the Stress-induced Transformation Behavior of Advanced High Strength Steel with Two-dimensional X-ray Diffraction (2D XRD)  
**B.M. Hance**, **A.A. Hall**, United States Steel Corporation-Automotive Center, Troy, MI, USA  
**D.P. Hoydick**, **L.D. Martin**, **B.R. Strohmeier**, United States Steel Corporation-Research and Technology Center, Munhall, PA, USA
- 11:20 D-81 MYTHEN2 R 2D Detector for Residual Stress Applications Using Laboratory Robots and Diffractometers  
**D. Murer\***, **Ch. Hörmann**, DECTRIS Ltd, Baden, Switzerland  
**L. Suominen**, **H. Larjosuo**, **J. Wartiainen**, Stresstech Oy, Jyväskylä, Finland

### Applied Materials II

Lasalle B

Chairs: **T. Fawcett**, **T. Blanton**, ICDD, Newtown Square, PA, fawcett@icdd.com; tblanton@icdd.com

- 8:30 D-79 Invited - Single Crystal Structure Analysis of Designer Drugs Circulating in the Japanese Drug Market by the Synchrotron Radiation X-ray Diffraction  
**T. Hashimoto**, **N. Yasuda**, **N. Mizuno**, **S. Honda**, **S. Kimura**, Japan Synchrotron Radiation Research Institute/SPring-8, Hyogo, Japan  
**R. Hanajiri**, National Institute of Health Sciences, Japan  
**S. Hayakawa**, SPring-8 and Hiroshima University, Japan  
**Y. Nishiwaki**, SPring-8 and Kochi University, Japan
- 9:00 D-88 Linear Diblock Copolymer Micellization Kinetics Probed by Integrated Microfluidic Device and Small-angle X-ray Scattering  
**J. Kalkowski\***, **C. Liu**, **P. Leon-Plata**, **M. Szymusiak**, **Y. Liu**, University of Illinois at Chicago, Chicago, IL, USA  
**W. Shang**, **S. Chakravarthy**, **T.C. Irving**, Illinois Institute of Technology, Chicago, IL, USA  
**S.V. Kathuria**, **O. Bilsel**, University of Massachusetts Medical School, Worcester, MA, USA

9:20	D-35	Investigating Crystal Structure, Preferred Orientation, and Disorder in Poly(Ethylene Furanoate) Using X-ray Fiber Diffraction <b>Y. Mao</b> , University of Maryland and National Institute of Standards and Technology, College Park, MD, USA <b>D. Bucknall</b> , Heriot-Watt University, Edinburgh, UK <b>R. Kriegel</b> , The Coca-Cola Company, Atlanta, Georgia, USA
9:40	D-13	Temperature Dependency of Morphological Structure of Thermoplastic Polyurethane using WAXS and SAXS <b>S.Witzleben, K.Walbrück</b> , Bonn-Rhein-Sieg University of Applied Sciences, Rheinbach, Germany
10:00		<b>Break</b>
10:20	D-57	Evolution of Carbon Fiber Microstructure During Carbonization and High-Temperature Graphitization Measured In Situ Using Synchrotron Wide-Angle X-ray Diffraction <b>M.J. Behr, B.G. Landes, B.E. Barton, G.F. Billovits, E.J. Hukkanen, J.T. Patton</b> , The Dow Chemical Company, Midland, MI, USA <b>J.E. Rix, D.T. Keane, S.J. Weigand</b> , Northwestern University, Argonne, IL, USA
10:40	D-86	X-ray Quantification of Phospholipid Monolayer Structural Changes <b>P. Zhang*, A. Donovan, J. Kalkowski, C. Liu, Y. Liu, M. Schlossman</b> , University of Illinois at Chicago, Chicago, IL, USA <b>W. Bu, B. Lin</b> , University of Chicago, Chicago, IL, USA
11:00	S-43	Fluorescence Plus Diffraction Mapping of Tooth Tissues <b>S.R. Stock*, A. Telser</b> , Northwestern University, Chicago, IL, USA <b>L.F. Finney, E. Maxey, S. Vogt, J.S. Okasinski</b> , Argonne National Laboratory, Argonne, IL, USA

## Quantitative Analysis

**Lasalle C**

Chair: **L.L. Brehm**, Dow Chemical Company, Midland, MI, USA, llbrehm@dow.com

8:30	F-40	Invited - Rapid and Accurate Determination of Iron in Vitamins and Supplements via XRF <b>P. Palmer, S. Chew, J. Castillo, A. Lam</b> , San Francisco State University, San Francisco, CA, USA
9:00	F-26	Invited - When is Accreditation and Quality Assurance Systems Not Enough to Guarantee Accurate Analysis? <b>M. Loubser</b> , PPC Ltd., Johannesburg, Gauteng, South Africa
9:30	F-5	Combining Specimen Preconcentration and Ion Exchange Chromatography to Quantify Gallium and Trace Uranium in Plutonium Using WDXRF and Polarized EDXRF <b>C.G. Worley</b> , Los Alamos National Laboratory, Los Alamos, NM, USA
9:50	F-44	Analysis of Nanocone Arrays by Total Reflection X-ray Fluorescence <b>M. Schmeling</b> , Loyola University Chicago, Chicago, IL, USA <b>K. Steeves Lloyd, I.L. Bolotin, L. Hanley, I.V. Veryovkin</b> , University of Illinois at Chicago, Chicago, IL, USA
10:10		<b>Break</b>
10:30	F-14	Invited - Quantitative Analysis for the PIXL Mars2020 Micro-XRF Instrument <b>W.T. Elam*</b> , <b>L. O'Neil</b> , APL, University of Washington, Seattle, WA, USA
11:00	F-17	Superconducting Microcalorimeters for X-ray Spectroscopy <b>J. Fowler, D. Swetz, J. Ullom</b> , NIST, Boulder, CO, USA
11:20	F-12	Fundamental Parameter Models Encounter the Geometry of an EDXRF Setup <b>J. Heckel</b> , SPECTRO Analytical Instruments GmbH, Kleve, Germany
11:40	F-41	hiRX Field Testing Results Demonstrating New Elemental Analysis Capabilities <b>K.G. McIntosh*, G.J. Havrilla</b> , Los Alamos National Laboratory, Los Alamos, NM, USA <b>R.F. Gilmore, Jr., M.K. Holland</b> , Savannah River National Laboratory, Aiken, SC, USA

Chair: **K. Janssens**, University of Antwerp, Antwerp, Belgium, koen.janssens@uantwerpen.be

- 8:30 S-58** Invited - Spectromicroscopy Instrumentation and Techniques with Synchrotron and Laboratory X-ray Sources  
**S. Hayakawa**, Hiroshima University, Higashi-hirohsima, Hiroshima, Japan
- 9:00 F-31** Invited - Three Dimensional Imaging at the P06 Hard X-ray Micro/Nano-Probe  
**J. Garrevoet, U. Boesenberg, C.G. Schroer, G. Falkenberg**, DESY, Hamburg, Germany
- 9:30 S-53** Invited - Collimating Channel Arrays for 3D Micro Confocal X-ray Fluorescence  
**D. Agyeman-Budu**, Cornell University, Ithaca, NY, USA  
**S. Choudhury**, University of Saskatchewan, Saskatoon, SK, Canada  
**I. Coulthard, E. Hallin**, Canadian Light Source, Saskatoon, SK, Canada  
**R. Gordon**, Simon Fraser University, Burnaby, BC, Canada
- 10:00** Break
- 10:20 S-23** X-ray Polarization Analysis with Gas-Filled Microchannel Plates: GF-MCP  
**J.B. Wang, A. Mane, S. Liao, R. Wagner, J. Elam, D. Haskel**, Argonne National Laboratory, Lemont, USA
- 10:40 S-56** Characterization of Reflection Gratings by GIXRF and their Application as Amplitude Beam Splitter for the 4 – 13 keV X-ray Energy Range  
**D. Eichert, W. Jark**, Elettra - Sincrotrone Trieste, Basovizza, Trieste, Italy
- 11:00 D-63** Monitoring Performance of X-ray Mirrors and Diffracting Crystals without Detection of the Reflected X-rays  
**S. Stoupin**, Advanced Photon Source, Lemont, IL, USA
- 11:20 S-57** The X-ray Fluorescence Beamline at Elettra – Sincrotrone Trieste: New Characterization Opportunities for Nano-Structured Materials  
**D. Eichert, F. Brigidi, A. Gambitta, W. Jark**, Elettra - Sincrotrone Trieste, Basovizza, Trieste, Italy  
**L. Luehl**, Technische Universitaet Berlin, IOAP, Berlin, Germany

# 2016 DXC Program-at-a-Glance

Rooms	Lasalle A	Lasalle B	Lasalle C	Madison	Lakeshore A
Monday Morning Workshops ♦ 9:00 am – 12:00 Noon					
XRD			Basic to Intermediate XRD I (Rodriguez)	Diffraction Contrast Imaging (Patterson)	
XRF	Basic XRF (Drews)				
Special Topics		Synergies between Lab. & Synchrotron X-ray Methods (Seidler)			Fundamentals of X-ray Absorption (Bunker)
Monday Afternoon Workshops ♦ 1:30 – 4:30 pm					
XRD			Basic to Intermediate XRD II (Rodriguez)		Rietveld for Beginners (Toby/Von Dreele)
XRF	Energy Dispersive XRF (Lemberge)	Trace Analysis (Wobraushek/Strelj)			
Monday Evening XRD Poster Session & Reception 5:00 – 7:00 pm. (Michigan Room)					
Tuesday Morning Workshops ♦ 9:00 am – 12:00 Noon					
XRD				Structure Solution I (Kaduk//Papoula)	Two-dimensional Detectors (Blanton/He)
XRF	Micro XRF (Havrilla)	Quantitative Analysis I (Elam)			
Special Topics			Amorphous & Disordered Mats. I (Fawcett)		
Tuesday Afternoon Workshops ♦ 1:30 – 4:30 pm					
XRD				Structure Solution II (Kaduk/Papoula)	Advanced Rietveld (Toby/VonDreele)
XRF	XRF Sample Prep (Anzelmo)	Quantitative Analysis II (Elam)			
Special Topics			Amorphous & Disordered Mats. II (Fawcett)		
Tuesday Evening XRF Poster Session & Reception 5:00 pm – 7:00 pm. (Michigan Room)					
Wednesday Morning Plenary Session ♦ 8:30-12:00 Imaging at Current and Next Generation Synchrotrons (Toby) (Lasalle)					
Wednesday Afternoon Sessions					
XRD		High Energy X-ray Microscopy (Almer/Stock)			
XRF			Trace Analysis (Zaitz/Martin)		BioXRF: Biomedical Applications
Special Topics	New Devel. in XRD/XRF Instr. I (Blanton/Fawcett)			X-ray Imaging I (Havrilla/Behr/Denecke)	
Wednesday Evening Vendor Sponsored Reception 5:30 pm – 7:00 pm. (Grand Ballroom – Exhibit Hall)					
Thursday Morning Sessions					
XRD		Rietveld (Lapidus)			
XRF			Industrial Apps (Broton)		BioXRF: Plant/Environmental/Microbial Science
Special Topics	New Devel. in XRD/XRF Instr.II (Blanton/Fawcett)			Cultural Heritage (Van Grieken)	
Thursday Afternoon Sessions					
XRD		Applied Materials I (Fawcett/Blanton)	General XRD (Murray)		
XRF	General XRF (Schmeling)				BioXRF: Related Technique & Methods Development
Special Topics				X-ray Imaging II (Havrilla/Behr/Denecke)	
Friday Morning Sessions					
XRD	Stress (Watkins)	Applied Materials II (Fawcett/Blanton)			
XRF			Quantitative Analysis (Brehm)		
Special Topics				X-ray Optics (Janssens)	



## PPXRD-14

Pharmaceutical Powder X-ray Diffraction Symposium  
XRD Training for the Pharmaceutical  
Scientist



### Sanibel Harbour Marriott

Fort Myers, FL  
6 – 9 June 2016

[www.icdd.com/ppxrd](http://www.icdd.com/ppxrd)

## SESSIONS...

- Patent Issues
- Amorphous, Activated, and Nano Materials
- Qualitative and Quantitative Analysis
- PXRD Techniques/Crystal Structure Prediction/Crystal Structure Verification
- New Frontiers in X-ray Diffraction for Pharmaceutical R&D
- Complementary Techniques/Formulation & Product Development

Visit ICDD's website links that demonstrate polymorph analyses, clustering analysis for crystallinity, crystallite size determinations, and Rietveld analysis using this database.

- PDF-4/Organics: [www.icdd.com/products/pdf4-organics.htm](http://www.icdd.com/products/pdf4-organics.htm)
- ICDD Tutorials: [www.icdd.com/resources/tutorials/](http://www.icdd.com/resources/tutorials/)
- PPXRD Presentations: [www.icdd.com/ppxrd/ppxrd-presentations.htm](http://www.icdd.com/ppxrd/ppxrd-presentations.htm)

Sponsored by



**Celebrating 75 Years Serving  
the Scientific Community**

[marketing@icdd.com](mailto:marketing@icdd.com)



ICDD, the ICDD logo and PDF are registered in the U.S. Patent and Trademark Office.  
Powder Diffraction File is a trademark of JCPDS—International Centre for Diffraction Data  
©2016 JCPDS—International Centre for Diffraction Data - 1/16

# SUCCESS

is being excellent at what you do

Join ICDD at our free PDF-4 Users' Meeting  
before the 65<sup>th</sup> Annual Denver X-ray Conference!

## • Users' Meeting

Sunday, 31 July 2016

Denver X-ray Conference 2016 • Rosemont, Illinois

10:00 am–4:00 pm

Register by 22 July 2016

Participants are encouraged to bring their laptops to this workshop. ICDD will install a trial version of the PDF-4+ to facilitate a hands-on workshop.

## • Getting Started Tutorial

This tutorial will discuss and demonstrate the basic functions of PDF-4 data mining, thus enabling the user to distill the huge number of entries in PDF-4 to a manageable selected subset.

- Selecting search criteria for >65 unique Search Fields
- Viewing/analyzing search results
- Using History to optimize your searches
- Using digital patterns for data simulations and analysis

## • Advanced Features Tutorial

This tutorial focuses on the power of PDF-4 data mining and Sleve+ for phase identification, simulation of X-ray, neutron, and electron diffraction patterns, and retrieval/use of PDF-4 database information for advanced analyses.

- Performing neutron and electron diffraction simulated profiles, electron backscatter patterns (EBSD), selected area electron diffraction patterns (SAED), and ring patterns
- Advanced data mining — tools to extract the data you need
- Using Sleve+ — choosing the appropriate search criteria and strategies for identification and problem analysis
- Interfaces — Using PDF-4 information as input for advanced analyses (whole-pattern fitting, structure analysis, molecular visualization)
- Similarity indexes — their use and value
- How to choose entries with atomic coordinates for Rietveld Refinement

Learn how to get the most from your PDF-4 database from the database experts.

Register online at [www.icdd.com/education/usersmeeting.asp](http://www.icdd.com/education/usersmeeting.asp)



International Centre for Diffraction Data  
12 Campus Boulevard • Newtown Square, PA 19073  
Phone: 610.325.9814 • Toll-free (U.S. & Canada): 866.378.9331 • Fax: 610.325.9823  
[info@icdd.com](mailto:info@icdd.com) • [www.icdd.com](http://www.icdd.com) • [www.dxcicdd.com](http://www.dxcicdd.com)

# GRANT-IN-AID Program

**JOIN ICDD'S ELITE GROUP OF SCIENTISTS  
who contribute experimental powder diffraction patterns  
to the Powder Diffraction File™.**

**AS A MEMBER OF THIS ELITE GROUP, YOU WILL RECEIVE THE FOLLOWING BENEFITS:**

- Financial support to aid current research
- Publication of pattern(s) in the Powder Diffraction File (PDF)
- Receive calibration standards
- Purchase certain ICDD products at reduced prices
- Web-based access to the list of compounds in the ICDD master database—includes published patterns, as well as patterns still in the editorial process
- First-time grantees receive a complimentary one-year subscription to *Powder Diffraction*

For over 50 years, ICDD has supported a well-developed program of grants to researchers around the world. One of our main objectives is to expand the range of reference materials by producing and cataloging high-quality X-ray diffraction patterns in our internationally renowned database, the Powder Diffraction File. Thanks to the longevity of this program, these contributions account for approximately a quarter of the current experimental file. ICDD awards financial support to qualified investigators in the form of grant-in-aid on a competitive proposal basis. The duration of a grant is 12 months with two cycles per year. Cycle I begins 1 April and Cycle II begins 1 October.

## Distinguished Grantees



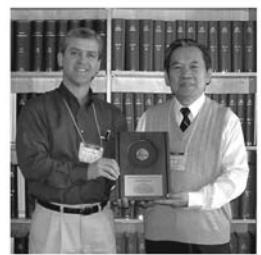
**2013**  
**Professor Xinkan Yao**



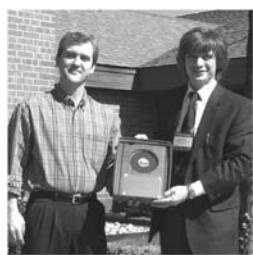
**2010**  
Dr. Tom Blanton  
presenting to  
**Professor Bogdan Lazoryak**



**2007**  
Dr. Miguel Delgado  
presenting to  
**Dr. Sergei Kirik**



**2004**  
Dr. Tom Blanton  
presenting to  
**Professor Shao-Fan Lin**



**2001**  
Dr. Tom Blanton  
presenting to  
**Professor Evgeny Antipov**



**1998**  
**Dr. Ekkehart Tillmanns**

**Geographic Locations of Grants  
for the Past 15 Years:**

- Argentina
- Austria
- Canada
- Chile
- Columbia
- Czech Republic
- France
- Germany
- India
- Israel
- Italy
- Japan
- Malaysia
- Netherlands
- P.R. of China
- Poland
- Portugal
- Russia
- Spain
- Switzerland
- Taiwan
- Tunisia
- Ukraine
- United Kingdom
- United States
- Uruguay

**Total Proposals Funded for the  
Past Fifteen Years: 699**



For more information on  
ICDD's Grant-in-Aid, visit  
[www.icdd.com/grants](http://www.icdd.com/grants)



**Celebrating 75 Years Serving  
the Scientific Community**



[www.icdd.com](http://www.icdd.com) | [marketing@icdd.com](mailto:marketing@icdd.com)

ICDD, the ICDD logo and PDF are registered in the U.S. Patent and Trademark Office.  
Powder Diffraction File is a trademark of JCPDS—International Centre for Diffraction Data  
©2016 JCPDS—International Centre for Diffraction Data - 1/16

## Characterization of Cultural Heritage Materials with the Powder Diffraction File

### ■ Phase identification

### ■ Conservation of artwork

### ■ Archaeological artifacts analysis

Identify minerals, metals, pigments, rocks, gemstones, ceramic inclusions, salt growths on glass, and more with the Powder Diffraction File, the most comprehensive materials diffraction database. X-ray diffraction provides a non-destructive method to perform characterization on materials of historical, artistic, and archeological significance.

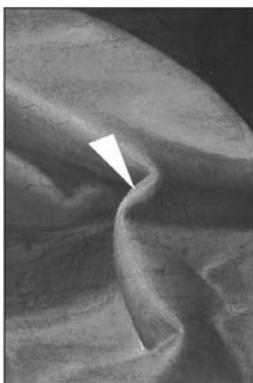


Figure 1. Madonna and Child by Giovanni Boltraffio's (Museum of Fine Arts, Budapest) – right: yellow area analyzed (photos Sarrazin).

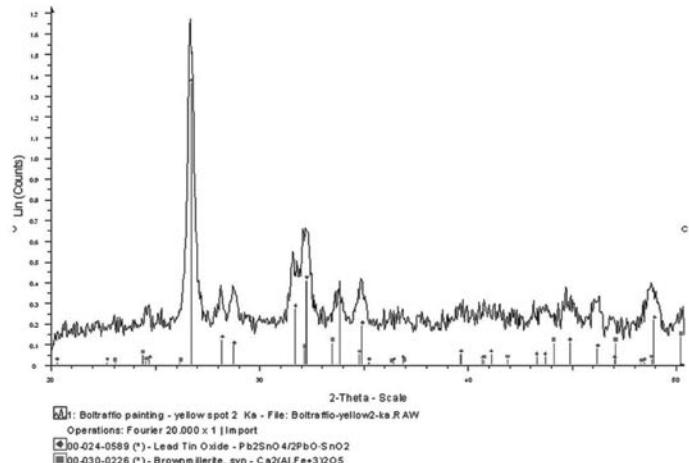


Figure 2. XRD data collected on Boltraffio's yellow – 50 min integration.

You can trust your analyses with the only crystallographic databases with quality marks and quality review processes that are ISO certified.

<b>S</b>	Standardized data
<b>M</b>	More coverage
<b>A</b>	All data sets are evaluated for quality
<b>R</b>	Reviewed, edited, and corrected prior to publication
<b>T</b>	Targeted for material identification and characterization

### The Powder Diffraction File (PDF®)

PDF-2 2015	278,503 material entries
PDF-4+ 2015	365,877 material entries
WebPDF-4+ 2015	365,877 material entries
PDF-4/Minerals 2015	42,852 material entries
PDF-4/Organics 2016	501,964 material entries

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

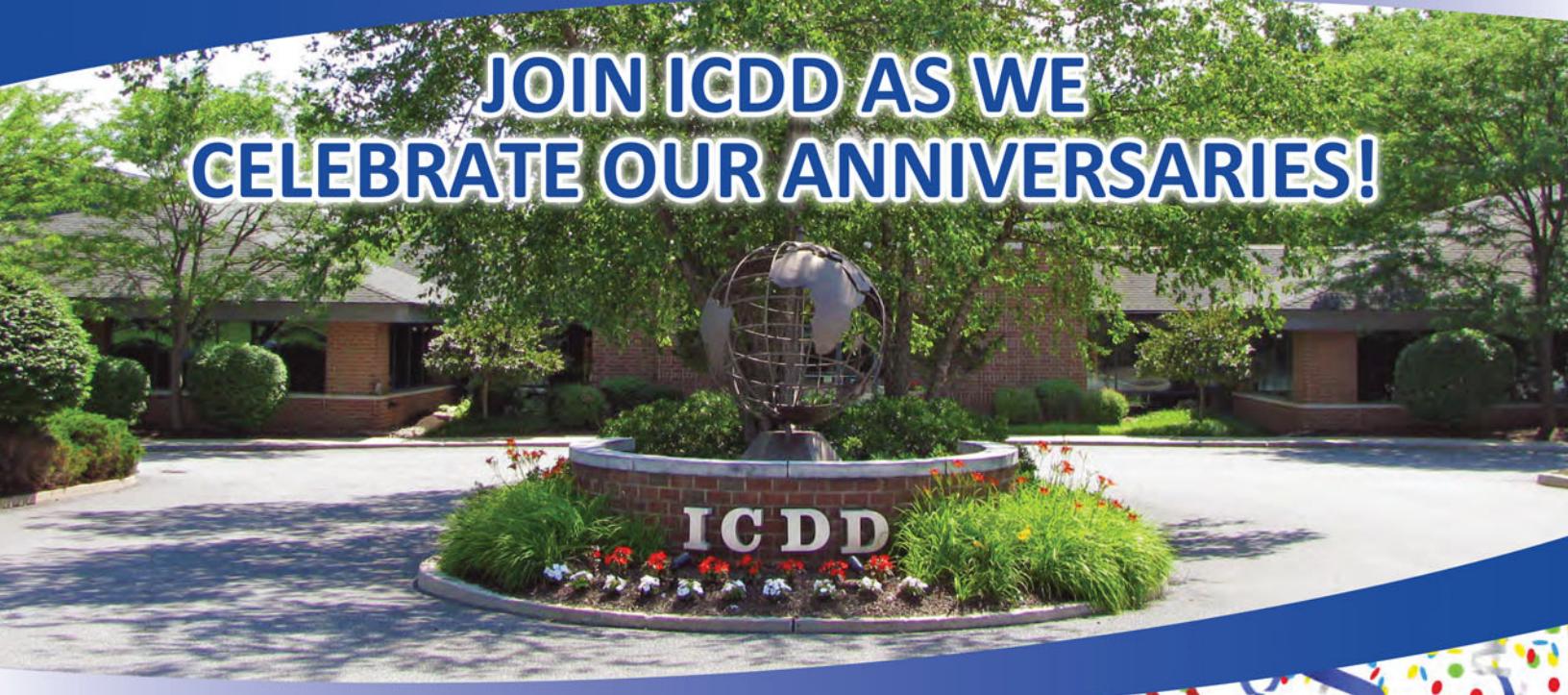
Figure 1-2. Advances in X-ray Analysis, Vol52; A PORTABLE NON-INVASIVE XRD-XRF INSTRUMENT FOR THE STUDY OF ART OBJECTS. P. Sarrazin, G. Chiari, M. Gailhanou. Copyright ©JCPDS—International Centre for Diffraction Data 2009 ISSN 1097-0002.



[www.icdd.com](http://www.icdd.com) | [marketing@icdd.com](mailto:marketing@icdd.com)

ICDD, the ICDD logo and PDF are registered in the U.S. Patent and Trademark Office. Powder Diffraction File is a trademark of JCPDS—International Centre for Diffraction Data. ©2016 JCPDS—International Centre for Diffraction Data – 5/16

# JOIN ICDD AS WE CELEBRATE OUR ANNIVERSARIES!



**75<sup>th</sup>**  
**Anniversary**  
*Serving the*  
**Scientific Community**

**65<sup>th</sup>**  
**Anniversary of**  
*Denver X-ray*  
**Conference**

**30<sup>th</sup>**  
**Anniversary of**  
*Powder Diffraction*

## About ICDD

We were established in 1941 as a non-profit scientific organization dedicated to collecting, editing, publishing, and distributing powder diffraction data for the identification of materials. The membership of the ICDD consists of worldwide representation from academe, government, and industry.

As we celebrate our 75th anniversary, we reflect on our founders' visions to serve as an organization dedicated to materials analysis and education. Our dynamic organization continues to evolve along with the community that it serves – from handwritten entries to data cards, keypunch cards, magnetic tape, CDs and DVDs, and now access via the Web. We will continue to be the world center for quality diffraction and related data. We will continue to promote the application of materials characterization methods in science and technology by providing forums for the exchange of ideas and information.

[WWW.ICDD.COM](http://WWW.ICDD.COM)



ICDD, the ICDD logo and PDF are registered in the U.S. Patent and Trademark Office. Powder Diffraction File is a trademark of JCPDS—International Centre for Diffraction Data ©2016 JCPDS—International Centre for Diffraction Data - 1/16

# Guidance software... makes powder diffraction easy

Automatic alignment, CBO, and SmartLab's Guidance software engine combine to create an extremely flexible, intelligence-based data collection platform. SmartLab gathers information about your sample, suggests measurement configurations, helps you set the diffractometer, and executes measurements, all with the help of user-friendly dialog screens. CBO technology allows simple selection of focusing and parallel beam geometries on demand for the widest possible range of applications.

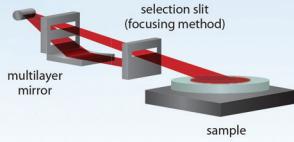
Supported powder diffraction applications include:

- Phase identification
- Quantitative analysis
- Percent crystallinity
- Crystallite size/lattice strain analysis
- Precise lattice parameter determination
- Rietveld refinement

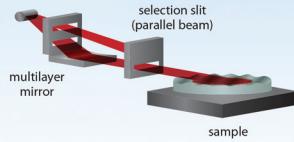
## Cross Beam Optical (CBO) technology

Change and adjust optics easily, whether you are using focusing optics in the direct beam path, or a multilayer mirror optic for high-brilliance, monochromated parallel beams.

Bragg-Brentano focusing

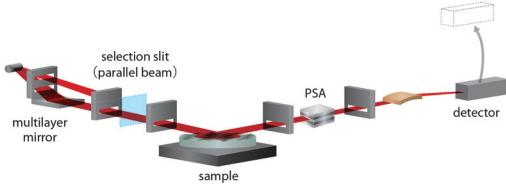


Parallel beam



## High resolution parallel beam optics

By combining the parallel beam from a multilayer mirror with a long slit PSA (parallel slit analyzer), you can obtain exceptionally accurate, high-resolution data with high repeatability without the influence of sample shape or measurement environment. The effectiveness of this configuration is particularly notable for in-situ analysis, powder structure determination, and the analysis of clay minerals and organic materials.



# improve your science

with the AXRD Benchtop Powder Diffractometer

FIND OUT WHY SO MANY SCIENTISTS  
ARE CHOOSING PROTO.

[www.protoxrd.com/powder](http://www.protoxrd.com/powder)



# PROTO

x-ray diffraction systems & services

For more information and to  
download our product catalog.



1-734-946-0974 [powder@protoxrd.com](mailto:powder@protoxrd.com)