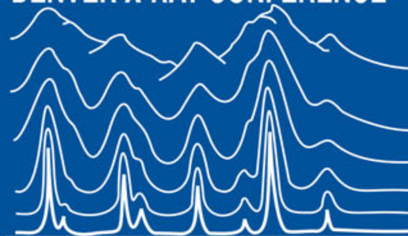
64th Annual Conference on Applications of X-ray Analysis

DENVER X-RAY CONFERENCE®



THE DENVER X-RAY CONFERENCE & TXRF 2015

• • •

Programs Now Available On-line

www.DXCICDD.com
www.DXCICDD/TXRF.com

Abstracts for poster presentation are still being accepted - submit on-line.

3 – 7 AUGUST 2015

The Westin Westminster, Westminster, Colorado, U.S.A.

Joint Conference with the 16th International Conference on Total Reflection X-ray Fluorescence Analysis and Related Methods (TXRF 2015)

Sponsored by

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DENVER X-RAY CONFERENCE ORGANIZING COMMITTEE

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

Cev Noyan, *Columbia University, New York, NY,* icn2@columbia.edu

Brian Toby, *Argonne National Laboratory, Advanced Photon Source, Argonne, IL,* brian.toby@anl.gov

Rene van Grieken, *University of Antwerp, Antwerp, Belgium,* rene.vangrieken@ua.ac.be

Mary Ann Zaitz, *IBM, Hopewell Junction, NY,* zaitz@us.ibm.com

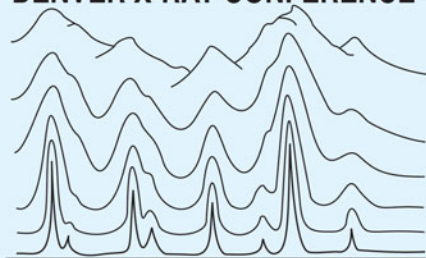
Denise Zulli, *ICDD, Newtown Square, PA,* zulli@icdd.com

MEMBERS EMERITUS:

Victor Buhrke, Portola Valley, CA

Clay Ruud, Spokane, WA

Future Conferences:



The **2016 Denver X-ray Conference** will be held at the Westin O'Hare Hotel, located on River Road in Rosemont, IL, the week of **August 1-5, 2016**.

The 2017 dates will be confirmed shortly, but DXC is planning to make a return to Big Sky in 2017!

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TABLE OF CONTENTS

WORKSHOPS

Monday Morning Workshops .... Page 4
- Basic to Advanced XRD Material Analysis I
- Structure Determination from Laboratory X-ray Powder Diffraction Data
- Basic XRF

Monday Afternoon Workshops................................ Page 5
- Basic to Advanced XRD Material Analysis II
- Fundamentals of Neutron Diffraction
- Energy Dispersive XRF
- Micro XRF

Tuesday Morning Workshops...............................Pages 6-7
- Stress
- Quantifying Crystalline & Amorphous Phases I
- Quantitative Analysis I
- Uncertainty in XRF

Tuesday Afternoon Workshops .... Page 8
- Synchrotron X-ray Coherent Diffraction Imaging and Ptychography
- Quantifying Crystalline & Amorphous Phases II
- Quantitative Analysis II
- Sample Preparation of XRF

POSTER SESSIONS

Poster Sessions
- Monday Evening XRD Poster Session............... **Pages 9-10**
- Tuesday Evening XRF Poster Session .... **Page 11**

ORAL SESSIONS

Wednesday Morning Session................................. Page 12
- Plenary Session: TXRF Around the World

Wednesday Afternoon Sessions....................... Pages 12-14
- New Developments in XRD/XRF Instrumentation
- Extremely Bright: The Future of X-ray Analysis
- Quantitative Analysis

Thursday Morning Sessions .... Pages 15-16
- Stress Analysis/Ptychography
- Applied Materials
- General XRF

Thursday Afternoon Sessions........................... Pages 17-18
- Energy Materials
- General XRD
- Environmental & Geological Applications

Friday Morning Sessions.................................. Pages 19-20
- Rietveld
- Micro XRF
- Fusion & Industrial Applications of XRF

PROGRAM-AT-A-GLANCE

Program-At-A-Glance.. Page 21
- Please visit the TXRF 2015 website to view the technical program of the 16th International Conference on Total Reflection X-ray Fluorescence Analysis and Related Methods: www.dxcicdd.com/txrf

View Program-at-a-Glance

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2015 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 Advanced XRD Material Analysis I — Standley I

Organizers & Instructors:
S.T. Misture, NYS College of Ceramics at Alfred University, Alfred, NY, misture@alfred.edu
T.N. Blanton, T.G. Fawcett, International Centre for Diffraction Data, Newtown Square, PA, tblanton@icdd.com; fawcett@icdd.com

Basic: An overview of the principles of diffraction from crystals will be followed by an analysis of the X-ray beam optics needed in powder diffraction experiments. Various sample and detector options will be surveyed, as well as optical components useful in some powder XRD measurements. Phase identification using XRD databases will be covered in detail, with emphasis on potential pitfalls, detection limits, and tips and tricks for difficult multi-phase problems. An overview of the physical and microstructural information that can be garnered from the peak locations, intensities and peak widths will be introduced in this morning session.

Advanced: The afternoon session will focus on the use of XRD for quantitative phase analysis, lattice parameter refinement for determination of solid solution compositions, and analysis of crystallite size and microstrain. A brief overview of structure determination from powder diffraction data will also be presented, capturing the main concepts in unit cell indexing and structure solution using ab-initio methods.

Structure Determination from Laboratory X-ray Powder Diffraction Data — Standley II

Organizer & Instructors:
A. Kern, Bruker GmbH, Karlsruhe, Germany, arnt.kern@bruker.com
I. Madsen, CSIRO Mineral Resources Flagship, Melbourne, Australia
P. Whitfield, Oak Ridge National Laboratory, Oak Ridge, TN, USA
J. Kaduk, Poly Crystallography Inc., Naperville IL, USA

Structure determination from laboratory powder data has developed rapidly over the last two decades as emphasised by the significant increase in the number of published structures solved in this way, both organic and inorganic. New developments in laboratory instrumentation (mostly detectors), methodology, and computing now allow determination of structures, the complexity of which is apparently only limited by the data quality at hand.

This workshop addresses beginners and intermediates. We will provide an overview about the currently available methodology for structure determination and discuss limitations inherent to laboratory data compared to data collected at synchrotron and neutron diffraction beamlines.

Basic XRF — Cotton Creek

Organizer & Instructors:
A.R. Drews, Ford Motor Company, Dearborn, MI, adrews@ford.com
G.J. Havrilla, Los Alamos National Laboratory, Los Alamos, NM

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.

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Basic to Advanced XRD Material Analysis II — Standley I

Organizers & Instructors:
S.T. Misture, NYS College of Ceramics at Alfred University, Alfred, NY, misture@alfred.edu
T.N. Blanton, T.G. Fawcett, International Centre for Diffraction Data, Newtown Square, PA, tblanton@icdd.com; fawcett@icdd.com

Continued from Monday morning

Fundamentals of Neutron Diffraction — Standley II

Organizer & Instructors:
P.S. Whitfield, Oak Ridge National Laboratory, Oak Ridge, TN, whitfieldps@ornl.gov
T.G. Fawcett, International Centre for Diffraction Data, Newtown Square, PA, fawcett@icdd.com
A. dos Santos, **J.R. Bunn**, Oak Ridge National Laboratory, Oak Ridge, TN
J. Faber, Faber Consulting Inc., Thornton, PA

Neutron diffraction is a powerful tool for materials analysis. Neutrons have many properties that make them ideal for certain types of analysis. For example a high sensitivity to hydrogen makes neutron diffraction ideal for the study of fuel cells, polymers and proteins. Neutron diffraction can be used to study the magnetic structure of materials. Worldwide neutron facilities are now available to a wide variety of scientists through general user proposals and mail in programs.

In this workshop we will explore the basics physics of neutron diffraction including the similarities and differences between neutron diffraction and X-ray diffraction. The various types of neutron diffractometers will be described, such as constant wavelength and time-of-flight, that can provide a range of high resolution and *in-situ* analyses. We will demonstrate a new phase identification system specifically developed for neutron diffraction analyses within the Powder Diffraction File™, PDF-4+ database. Finally, a review of material and structural analyses and applications will be shown.

Energy Dispersive XRF — Cotton Creek

Organizer & Instructors:
R. Phillips, Thermo Scientific, West Palm Beach, FL, rich.phillips@thermofisher.com
P. Lemberge, Thermo Scientific, Ecublens, Switzerland

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 instrumentation, components, and applicability of EDXRF; 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; and sample preparation. A variety of applications will be presented as real-life examples where EDXRF is being used to solve complex analytical problems. The major emphases will be applicability of EDXRF and the optimal protocol for generating and reporting of reliable experimental results.

Micro XRF — Meadowbrook

Organizer & Instructors:
G.J. Havrilla, Los Alamos National Laboratory, Los Alamos, NM, Havrilla@lanl.gov
S. Vogt, Advanced Photon Source, Argonne National Laboratory, Argonne, IL

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.

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Stress — Standley I

Organizer & Instructor:
I.C. Noyan, Columbia University, New York, NY, icn2@columbia.edu

This workshop is intended to introduce novice users to the basic techniques used in diffraction-based residual stress determination. Single exposure, $\sin^2(\text{psi})$, two-tilt and triaxial stress determination techniques will be introduced and instrumental errors associated with the measurement will be discussed. At the end of the seminar, the attendees should be able to evaluate the validity of a diffraction-based stress determination experiment.

Quantifying Crystalline and Amorphous Phases I — Standley II

Organizer & Instructors:
A. Kern, Bruker GmbH, Karlsruhe, Germany
I. Madsen, CSIRO Mineral Resources Flagship, Melbourne, Australia
M. Raudsepp, The University of British Columbia, Vancouver, Canada
P. Whitfield, Oak Ridge National Laboratory, Oak Ridge, TN

This workshop will discuss the basis of quantitative phase analysis (QPA) for both single peak and whole pattern approaches. The focus will be on how to select and apply these methods, particularly in the context of the derivation of absolute phase abundances. The presence of poorly crystalline or amorphous content requires extension of the basic methods, but once these are established, they can be shown to produce QPA to the similar lower limits of detection and accuracy as for crystalline phases. Worked examples for various methods will be presented using both mineralogical as well as pharmaceutical samples.

MORNING, 9:00 - 12:00: METHODOLOGY

- Basis: QPA of crystalline and amorphous phase abundance
- Methods for QPA
- Practical Assessment of Merits of Methods for QPA

AFTERNOON, 1:30 - 4:30: TOWARDS ONE WEIGHT PERCENT ACCURACY

- How to assess accuracy
- Minimising systematic errors
- Use of constraints and restraints

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Quantitative Analysis I — Cotton Creek

Organizer & Instructors:
M. Mantler, Rigaku Corporation, Japan, michael.mantler@rigaku.com
W.T. Elam, University of Washington, Seattle, WA
B. Vrebos, PANalytical, Almelo, The Netherlands
K. Kawakyu, Rigaku Corporation, Osaka, Japan

Note: While the general contents of the workshop remain similar to that of the previous years, the way of presentation has been re-structured:

- *to provide a smooth transition from the Monday workshop "Basic XRF";*
- *the mathematical part will be greatly reduced; instead a downloadable brochure is provided, which covers the mathematical background, as well as an Excel tool (add-in) with basic XRF-related functions and fundamental parameters. This should allow a more practical access to data evaluation on the participants' own laptops;*
- *to put a stronger focus at practical applications.*

Part I, Morning session: Basic Methods

- Classical fundamental parameters and mathematical models based on Excel add-ins to be used with personal (Windows) laptops.
- Empirical and theoretical influence coefficients.
- Compensation methods (standard addition, internal standard, heavy absorber, Compton scattering).
- Semi-quantitative analysis.

Part II, Afternoon session: Advanced Methods

- Fundamental parameter collections and tube spectra: Resources - availability, and reliability.
- Layered materials, inhomogeneous samples, rough surfaces, and light elements.
- Elaborate application examples.
- Questions and answers.

Uncertainty in XRF — Meadowbrook

Organizer & Instructors:
J. Kawai, Kyoto University, Kyoto, Japan, kawai.jun.3x@kyoto-u.ac.jp
S. Ichikawa, Meiji University, Kanagawa, Japan
U. Yasushi, Mitsubishi Electric Co., Hyogo, Japan

This workshop provides basic introduction how (i) the sample preparation (sample amount, particle size for e.g. rice as received or pulverized, pressure to make a briquette, glass bead components and thickness, specimen diameter, …); (ii) spectrometer settings (XRF intensity, A/D conversion gain, smoothing, background subtraction, dwelling time, iteration time, …); and (iii) measurement conditions (sample thickness, monochromatic X-ray energy, incident synchrotron X-ray beam angle, acceleration voltage in EPMA, …) will affect the results of quantitative and even qualitative results of XRF. Note: (i) is for laboratory or handheld XRF, (iii) for synchrotron and EPMA experiments, and (ii) for both.

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Synchrotron X-ray Coherent Diffraction Imaging and Ptychography — Standley I

Organizer & Instructors:
M.V. Holt, **R. Harder, D. Vine,** Argonne National Laboratory, Argonne, IL, mvholt@anl.gov

The use of phase coherence in synchrotron X-ray beams has created several novel imaging methods that are capable of quantifying materials properties at a spatial resolution well beyond that of the X-ray beam size. Coherent diffraction imaging (CDI) techniques, such as Ptychography use iterative algorithms to analyze experimentally observed coherent scattering patterns and reconstruct a high-resolution real-space visualization of the complex interaction between the beam and the sample. In transmission geometry these phase and amplitude shifts that are given to the beam by the sample are sensitive to internal density fluctuations and interfaces, whereas in Bragg geometry these shifts are also sensitive to subtle crystalline distortions, such as lattice strain or curvature. Reconstructed CDI visualizations may be produced in two and sometimes three dimensions, and frequently the properties of the X-ray beam itself can be determined along with the sample structure. Applications of these techniques are varied and becoming increasingly important with the advent of new high-brilliance synchrotron sources and source upgrades. This workshop will introduce the basic principles and survey current research topics in Coherent Diffraction Imaging and Ptychography.

Quantifying Crystalline and Amorphous Phases II — Standley II

Organizer & Instructors:
A. Kern, Bruker GmbH, Karlsruhe, Germany, arnt.kern@bruker.com
I. Madsen, CSIRO Mineral Resources Flagship, Melbourne, Australia
M. Raudsepp, The University of British Columbia, Vancouver, Canada
P. Whitfield, Oak Ridge National Laboratory, Oak Ridge, TN

Continued from Tuesday morning

Quantitative Analysis II — Cotton Creek

Organizer & Instructors:
M. Mantler, Rigaku Corporation, Japan, michael.mantler@rigaku.com
W.T. Elam, University of Washington, Seattle, WA
B. Vrebos, PANalytical, Almelo, The Netherlands
K. Kawakyu, Rigaku Corporation, Osaka, Japan

Continued from Tuesday morning

Sample Preparation of XRF — Meadowbrook

Organizer & Instructors:
J. Anzelmo, Anzelmo & Associates, Inc., Madison, WI, jaanzelmo@aol.com
M. Provencher, Corporation Scientifique Claisse, Quebec City, Quebec, Canada

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.

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XRD Poster Session – Monday Evening,
Westminster Foyer

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

Judge: T.R. Watkins, Oak Ridge National Laboratory, Oak Ridge, TN
Three "Best Poster" awards will be given at the end of the session, including "Best Student Poster".

**Signifies Presenting Author, when noted*

D-2 **Crystal Structures of Large-Volume Commercial Pharmaceuticals**
J.A. Kaduk, Poly Crystallography, Inc., Naperville, IL, USA
J.W. Reid, Canadian Light Source, Saskatoon, Canada
R. Papoular, Leon Brilouin Laboratory, Saclay, France
K. Zhong, **A.M. Gindhart**, ICDD, Newtown Square PA, USA

D-6 **Structural Study of the Ball-milled $Cr_{80}Co_{20}$ Alloy by the Rietveld Refinement of XRD profiles**
S. Louidi, University of Skikda, Skikda, Algeria
F.-Z. Bentayeb, University of Annaba, Algeria
J.J. Sunol, **L. Escoda**, University of Girona, Spain

D-13 **X-ray Analysis of Consumer Grade 3D Printer Materials**
S.A. Speakman, PANalytical Inc, Westborough, MA, USA

D-21 **Quick and High Sensitivity Measurement Combining 2D Hybrid Pixel Array Detector "HyPix-3000" and XRD-DSC**
C. Sato*, **A. Yamano**, **T. Konya**, Rigaku Corporation, Tokyo, Japan

D-29 **ONE SHOT Analysis using Wide-range High-speed Detector**
R. Ogawa*, **Y. Okamoto**, **H. Sekiguchi**, **H. Furukawa**, **K. Koyanagi**, Shimadzu Corporation, Kyoto, Japan
D. Davis, Shimadzu Scientific Instruments, Inc., MD, USA

D-31 **Quantitative Phase Analysis of Shale Cores Taken from the Sebree Trough in SW Ohio**
J. Cowen*, **J. Bloxson**, **B. Saylor**, Case Western Reserve University, Cleveland, OH, USA

D-34 **Optimized Clay Mineral Identification by X-ray Diffraction Analysis of Oriented Smear Slides**
J. Bentz, Queen's University, Kingston ON, Canada
J. Anderson, PANalytical, Montreal QC, Canada

D-36 **ICDD Powder Diffraction File™ Coverage of Polymers Used in Pharmaceutical and Biomedical Applications**
T. Blanton, **S. Gates**, **T. Fawcett**, ICDD, Newtown Square, PA, USA

D-39 **Monitoring of CoS_2 Reactions using High Temperature XRD Coupled with Gas Chromatography (GC)**
M.A. Rodriguez, **J.J.M. Griego**, **C.D. Mowry**, **A.S. Pimentel**, **T.M. Anderson**, Sandia National Laboratories, Albuquerque, NM, USA

D-40 **Crystal Structure, Chemistry and Evidence of Radiation-Induced Phase Transition in Monazite**
M.M. Zaman*, **S.M.Antao**, University of Calgary, Calgary, Alberta, Canada

D-44 **Relating Particle Sampling Statistics and Intensity Statistics in Powder Diffraction Experiments with Nanocrystalline Powders**
H. Öztürk*, **I.C. Noyan**, Columbia University, New York, NY, USA
H. Yan, **J. Hill**, BNL, Upton, NY, USA

D-46 **Enhancing PDF Data Quality on a Laboratory Powder Diffractometer**
T. Hartmann, STOE & Cie GmbH, Darmstadt, Germany

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D-48 **Diffraction Opportunities at the Spallation Neutron Source for Materials Research**
P.S. Whitfield*, **A. Huq**, ORNL, Oak Ridge, TN, USA

D-50 **Residual Stress Evaluation of Shot Peened Ag-based Contact Materials via Diffraction Technique**
S.-Y. Lee*, Columbia University, New York, NY, USA
H.-S. Lee, **M.-H. Lee**, Korea Institute of Industrial Technology, Incheon, Korea

D-54 **NIST Standard Reference Materials for X-ray Metrology**
J.P. Cline, **M. Mendenhall**, **D. Windover**, **A. Henins**, NIST, Gaithersburg, MD

D-55 **Structural Study of Polycrystalline Thin Layers of TiO_2 Prepared by Hydrothermal Synthesis**
S. Danis*, Charles University in Prague, Prague, Czech Republic
L. Matejova, Technical University of Ostrava, Ostrava, Czech Republic
M. Cerhova, Institute of Chemical Process Fundamentals of the CAS, Suchdol, Czech Republic

D-58 **Instrumental and Sample Based Error in Engineering Neutron Diffraction: Quantifying Total Error in Measured Strain**
J.R. Bunn, **A. Payzant**, **L.M. Kolbus**, **P.A. Cornwell**, Oak Ridge National Laboratory, Oak Ridge, TN, USA
I.C. Noyan, Columbia University, New York, NY, USA

D-61 **Beyond Phase Identification: Benchtop Diffractometers, Data Quality, and Applications**
N.L. Henderson, Bruker AXS, Inc., Madison, WI

D-62 **Structural Characterization of Reflectin-based Thin Films by Grazing Incidence X-ray Scattering**
Q. Lin, **K. Naughton**, **L. Phan**, **A.A. Gorodetsky**, University of California, Irvine, Irvine, CA
C. Zu, ALS - Lawrence Berkeley National Laboratory, Berkeley, CA

D-63 **The BTS 500 Benchtop Heating Stage: The First Commercial Non-Ambient XRD-Attachment For Benchtop Devices**
B. Puhr*, **A. Pein**, Anton Paar GmbH, Graz, Austria

D-64 **The TTK 600 Low-Temperature Chamber: A Novel Multipurpose Non-Ambient XRD Attachment**
B. Puhr*, **A. Pein***, Anton Paar GmbH, Graz, Austria

S-1 **Thickness Evaluation of Ultrathin Multiple High-k Films by X-ray Reflectivity and Electron Energy Loss Spectroscopy**
Y.-S. Yeh, **B.-C. He**, **W.-E. Fu**, **H.-C. Ho**, Industrial Technology Research Institute, Hsinchu, Taiwan

S-5 **Measurement of Residual Surface Damage in Single-Crystal Sapphire Wafer by X-ray Transmission Topography**
M.H. Choi, **C.S. Kim***, Korea Research Institute of Standards and Science (KRISS), Daejeon, Korea
H.-G. Jeon, **I.-Y. Jung**, **B.S. O**, Chungnam National University, Daejeon, Korea

S-9 **Achievement of Ultra-high Throughput with Vortex® Silicon Drift Detectors**
L. Feng, **S. Barkan**, **V. Saveliev**, **J. Wang**, **E. Damron**, HHSUS, Northridge, CA, USA

S-13 **A Small Angle X-ray Scattering Study of the Structural Changes and Thermal Stability of Highly Ordered Mesoporous Nanostructures**
Y. Kim*, **K. Park**, **Y.-H. Jung**, **G.-S. Hong**, **K. Han**, Korea Institute of Energy Research, Daejeon, Republic of Korea
G. Kwak, Korea Research Institute of Chemical Technology, Daejeon, Republic of Korea

S-17 **The Study of Nano-Fragmentary Materials for New X-ray Standard Reference Materials**
B. Kodess, ICS&E-VNIIMS, Moscow, Russian Federation
P. Kodess, ICS&E Aurora, Colorado, USA

S-21 **Completely Non-Destructive High-Resolution XRD Analysis of Cultural Heritage Objects**
G.M. Hansford*, **S.R. Turner**, **N. Karim**, **J. Hall**, University of Leicester, Leicester, UK

S-25 **The Vertically Aligned ZnO/Si-nanopillars with High Emission Property for the Applications of the X-ray Tube**
P.H. Kao, Industrial Technology Research Institute, Hsinchu, Taiwan
Y.M. Chang, **J.Y. Juang**, National Chiao Tung University, Hsinchu, Taiwan

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XRF and TXRF Poster Session – Tuesday Evening,
Westminster Foyer

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

Judges: **D. Broton**, Construction Technology Labs, Skokie, IL
J. Anzelmo, Anzelmo & Associates, Inc., Madison, WI
Three "Best Poster" awards will be given at the end of the session, including "Best Student Poster".

**Signifies Presenting Author, when noted*

F-4 **X-ray Fluorescence Analysis with Micro-glass-beads using One-milligram of Archaeological Ceramics for Application to Determination of Minor Elements**
S. Ichikawa*, **T. Nakamura**, Meiji University, Kanagawa, Kawasaki, Japan

F-9 **Elemental Characterization of Airborne Particulate Matter Collected Within The Canadian National Air Pollution Surveillance (NAPS) Program**
V. Celo*, **E. Dabek-Zlotorzynska**, **D. Mathieu**, Environnement Canada, Ottawa, Ontario, Canada

F-13 **Evaluating EDXRF Measurements of Atmospheric Aerosols with Multi-Elemental Reference Materials**
S. Yatkin, **K. Trzepla***, **W. White**, **N. Hyslop**, University of California, Davis, CA, USA

F-14 **Development of Single-Compound XRF Calibration Standards on PTFE Filters for Analysis of Aerosol Samples**
S. Yatkin, **K. Trzepla***, **W. White**, **N. Hyslop**, Univerity of California, Davis, CA, USA

F-20 **Challenge of Small Sample Analysis for Pharmaceutical Products and Food using Theoretical Scattered X-rays**
H. Furukawa*, **N. Ichimaru**, **S. Watanabe**, **K. Suzuki**, **M. Nishino**, **H. Ochi**, Shimadzu Corporation, Kyoto, Japan
D. Davis, Shimadzu Scientific Instruments, Inc., MD, USA

F-31 **New High Performance Digital Pulse Processor**
E. Lechner, **S. Pahlke**, **A. Pahlke**, **R. Fojt**, **J. Knobloch**, **C. Luckey**, KETEK GmbH, Munich, Germany

F-39 **Edge Absorption Non-Dispersive XRF (EA-NDXRF)**
J. Van Wagoner*, **S. Cornaby**, **S. Kamtekar**, Moxtek, Inc., Orem, UT, USA

F-40 **Educational XRF Kit**
S.W. Cornaby, **J. Van Wagoner**, **S. Kamtekar**, Moxtek Inc., Orem, UT, USA

F-43 **Theory of Polarization X-ray Fluorescence Intensity**
J. Kawai, Kyoto University, Kyoto, Japan

F-47 **Improvement of Spatial Resolution of Confocal Micro-XRF Images using Principal Component Analysis**
T. Matsuno, **Y. Kitado**, **M. Yamanashi**, **K. Tsuji**, Osaka City University, Osaka, Japan
T. Hasegawa, Kyoto University, Kyoto, Japan

F-48 **Secondary Excitation Observed in Lateral Scan using Confocal Micro-XRF**
K. Tsuji*, **T. Matsuno**, **Y. Takimoto**, Osaka City University, Osaka, Japan
N. Kawahara, Rigaku Corporation, Osaka, Japan

F-55 ***In vivo* L XRF Feasibility Studies of Uranium using ^{125}I Radioisotope**
K.R. Veeranki*, **D.R. Chettle**, **K.P. Timmaraju**, **E.D. Desouza** , McMaster University, Hamilton, ON, Canada
J. O'Meara, University of Guelph, Guelph, ON, Canada

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Plenary Session – Wednesday Morning, 8:30 AM – 11:45 AM
Standley Ballroom

Plenary Session: TXRF Around the World
Chair: Mary Ann Zaitz, IBM, Hopewell Junction, NY, USA

8:30 **Opening Remarks:**
Chairman of the Denver X-ray Conference, **W. Tim Elam**, University of Washington APL, Seattle, WA, USA

Presentation of Awards:
2015 Barrett Award to **Brian Toby**, Advanced Photon Source, Argonne National Laboratory, Argonne, IL
Presented by **Jim Kaduk**, Poly Crystallography Inc., Naperville, IL

2015 Jenkins Award to **Cev Noyan**, Columbia University, New York, NY, USA
Presented by **Tom Blanton**, International Centre for Diffraction Data, Newtown Square, PA, USA

2015 Jerome B. Cohen Student Award
The winner will be announced at the session. Presented by **Cev Noyan**, Columbia University, New York, NY, USA

Plenary Session Remarks by the Session Chair, **Mary Ann Zaitz**, Hopewell Junction, NY, USA

9:00 **T-3** Worldwide Distribution of TXRF - Its Capacity and Acceptance
Reinhold Klockenkämper, ISAS, Dortmund, Germany

9:45 **Break**

10:15 **T-10** Total Reflection X-ray Fluorescence in Latin America
Cristina Vázquez, University of Buenos Aires, Argentinean Atomic Energy Commission, Buenos Aires, Argentina

11:00 **T-33** Industrial Applications and Standardization of TXRF
Yoshihiro Mori, Horiba, Ltd., Kyoto, Japan

Oral Sessions – Wednesday Afternoon

**Signifies Presenting Author, when noted*

New Developments in XRD & XRF Instrumentation — Standley I

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

1:30 **D-25** The STOE STADI P with Ag K α_1-radiation – Highest Versatility for XRD and PDF
T. Hartmann, STOE & Cie GmbH, Darmstadt, Germany

1:40 **S-7** Current Status of the Liquid-Metal-Jet X-ray Source Technology
E. Espes*, **B.A.M. Hansson**, **O. Hemberg**, **M. Otendal**, **T. Tuohimaa**, **P. Takman**, Excillum AB, Kista, Sweden

1:50 **D-37** New Capabilities for Analysis of Organic Materials Using the ICDD PDF-4/Organics Database
S. Kabekkodu*, **S. Gates**, **A. Gindhart**, **E. Foster**, **M. Rost**, **M. Hammock**, **T. Blanton**, ICDD, Newtown Square, PA, USA

2:00 **D-42** TTK 600 Low-Temperature Chamber and BTS 500 Benchtop Heating Stage: Innovative Non-Ambient XRD Attachments for Material Investigations Under Multiple Environmental Conditions
A. Pein*, **B. Puhr**, Anton Paar GmbH, Graz, Austria

2:10 **S-10** Structural Examination of Physically Crosslinked Fluorinated Polyphosphazene Elastomers via Small Angle X-ray Scattering on a Multi-purpose Diffractometer
T. Modzelewski, **N.M. Wonderling**, **H.R. Allcock**, The Pennsylvania State University, University Park, PA, USA

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2:20 **S-6** On the Intensity of L-Line Due To Polarization
J. Kawai, **S. Imashuku**, **S. Akiba**, Kyoto University, Kyoto, Japan

2:30 **S-15** A New Method for Copper Concentrate Analysis Utilizing Fusion XRF
B.J. McBain, IMP Automation Ltd., Oakville, Ontario, Canada
R.D. Wilson, IMP Group Pty Ltd., Perth, Australia

2:40 **F-10** The New Generation of TheOx® Instrument from Claisse®
C. Audet, Claisse, Québec, QC, Canada

2:50 **S-14** Environmental Protection Considerations for X-ray Sources & Sensors
M. Wolf, Materion Electrofusion, Fremont, CA, USA

3:00 **Break**

3:20 **F-6** Improved Performance of Silicon Drift Detectors
A. Pahlke, **M. Bachmann**, **T. Eggert**, **R. Fojt**, **M. Fraczek**, **L. Höllt**, **M. Hofmann**, **P. Iskra**, **J. Knobloch**, **N. Miyakawa**, **S. Pahlke**, **J. Rumpff**, **O. Scheid**, **A. Simsek**, **I. Wennemuth**, KETEK GmbH, Munich, Germany

3:30 **D-22** Large-Area CdTe Pixel Detectors for X-ray Diffraction Applications
T. Donath, **M. Mueller***, **S. Commichau**, **V. Radicci**, **M. Rissi**, **T. Sakhelashvili**, **M. Schneebeli**, **C. Schulze-Briese**, **C. Broennimann**, DECTRIS Ltd., Baden, Switzerland

3:40 **F-51** Gas Sealed Low Energy Parallel-Plate Detector with Ultra-thin Window
A. Stratilatov, **R. Creigton**, **J. Barron**, **B. Harris**, Moxtek, Inc. Orem, UT, USA
D. Khazins, Independant Consultant, Madison, WI, USA

3:50 **D-45** A New Energy-Dispersive Position Sensitive Detector for XRD
B. Jones*, **J. Giencke**, Bruker AXS, Madison, WI, USA
A. Kern, Bruker AXS, Karlsruhe, Germany

4:00 **F-19** Development of the Novel WDXRF Apparatus into which Assembled DCCs and an SDD for Simultaneous Analyses on Multi Elements
T. Omori*, **K. Kohmoto**, **H. Ishii**, **K. Taniguchi**, Techno-X Co., Ltd., Osaka, Japan

4:10 **S-16** XRF Slurry Immersion Probe with 50 MM^2 SDD
B. Crosby, **A. Chowles**, **S. Liemar**, **C. Ming**, **H. Mao**, **H. Zeng**, **P. Hayles**, **M. Rose**, **T. Shah**, Thermo Fisher Scientific, Adelaide, SA, Australia
T. Strombotne*, Thermo Fisher Scientific, Longmont, CO, USA

4:20 **S-12** The Zetium X-ray platform with SumXcore Technology – New Analytical Possibilities
C. Tsouris, **A. Komelkov**, **F. Casco-Tañeza**, PANalytical BV, Almelo, The Netherlands

4:30 **F-24** Advances in Energy-Dispersive X-ray Fluorescence Spectrometry - The New S2 PUMA
F. Portala, **K. Behrens**, Bruker AXS, Karlsruhe, Germany
D. Pecard*, **A. Buman**, Bruker AXS, Madison, WI, USA

Extremely Bright: The Future of X-ray Analysis — Standley II

Chairs: **S. Vogt**, X-ray Science Division, Argonne National Lab, Argonne, IL, USA, svogt@aps.anl.gov
C.E. Murray, IBM T.J. Watson Research Center, Yorktown Heights, NY, USA, conal@us.ibm.com

2:00 Invited - Emerging *in-situ* Tools for X-ray Nanoprobe Investigations of Energy Materials at the Advanced Photon Source
T. Buonassisi, MIT, Photovoltaic Research Laboratory, Cambridge, MA, USA

2:30 **D-3** Invited - Defect Analysis at the Atomic Scale
F. Hofmann*, University of Oxford, Oxford, UK

3:00 **F-18** High Flux X-ray Beam Delivery System
W. Yun*, **J. Kirz**, **D. Reynolds**, **S. Chen**, **I. Spink**, **B. Stripe**, **S.J.Y. Lewis**, **A. Lyon**, Sigray, Inc., Concord, CA, USA

3:20 **Break**

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3:40 **F-58** Invited - X-ray Imaging of Whole Catalyst Particles - Prospects and Challenges
F. Meirer, Utrecht University, Utrecht, The Netherlands

4:10 **F-28** Combined Elemental XRF and Phase XRD Analyses of a Meteorite
F. Casco-Tañeza, **T. Witzke**, **N. Norberg**, PANalytical BV, Almelo, The Netherlands

4:30 **F-54** Encapsulated Ag-Hg XRF Calibration Standards for Mercury
V. Jaggi, **R.R. Pandey**, **N. Kumar**, Micromatter Technologies Inc., Vancouver, Canada

4:50 **F-32** Exploring the Future of Nanoelectronics using X-rays
C.E. Murray, IBM T.J. Watson Research Center, Yorktown Heights, NY, USA

Quantitative Analysis — Cotton Creek

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

1:20 **F-23** Invited - Seed Treatment Active Loadings and Single Seed Screening by X-ray Fluorescence
W.W. Brubaker, DuPont Corporate Center for Analytical Sciences, Wilmington, DE, USA

1:50 **F-12** Invited - Multimineral and Porosity Modeling using High-resolution XRF Core Scanning
W.C. Ingram, Weatherford Labs, Golden, CO, USA

2:20 **F-35** Bauxite Mineral Quantification using a Combined XRD and XRF Method
S.H. Nettles, CTL Group, Skokie, IL, USA

2:40 **F-52** KXRF Studies of Mercury in Kidney and Bone Phantoms
K.P. Timmaraju*, **D. Chettle**, **A. Armstrong**, **K.R. Veeranki**, McMaster University, Hamilton, ON, Canada

3:00 **Break**

3:30 **F-46** Quantitative Analysis Using PIXL, the Planetary Instrument for X-ray Lithochemistry
W.T. Elam, University of Washington, Seattle, WA, USA
A.C. Allwood, **M. Foote**, **R. Hodyss**, **E. J. Knowles**, **D.R. Thompson**, **L. Wade**, NASA Jet Propulsion Laboratory, Pasadena, CA, USA
D.T. Flannery, Caltech/NASA Jet Propulsion Laboratory, Pasadena, CA, USA
B. Clark, Space Sciences, Inc., Denver, CO, USA
J. Hurowitz, State University of New York at Stony Brook, Stony Brook, NY USA

3:50 **S-8** C/H and O Correction by a Scattered X-ray Internal Standard for XRF Analysis of Oils
K. Kawakyu*, **A. Morikawa**, **K. Watanabe**, **Y. Yamada**, **Y. Kataoka**, **M. Mantler**, Rigaku Corporation, Takatsuki, Osaka, Japan

4:10 **F-11** Analysis of Commercial Magnesium Stearate Products using XRF and ICP-OS Spectroscopy
S. Mamedov, **H. Savadkouei**, Horiba Scientific, Edison, NJ, USA

4:30 **F-44** Invited - Steps in the Quantification Procedure in XRF by a Versatile Software
P. Wobrauschek, **B. Grossmayer**, **H. Hable**, **C. Streli**, TU Wien, Vienna, Austria

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Oral Sessions – Thursday Morning

**Signifies Presenting Author, when noted*

Stress Analysis/Ptychography — Standley I

Chairs: **T.R. Watkins**, Oak Ridge National Laboratory, Oak Ridge, TN, watkinstr@ornl.gov
M.V. Holt, Center for Nanoscale Materials, Argonne National Lab, Argonne, IL, mvholt@anl.gov

8:30 **S-24** Invited - Digital Image Correlation and Neutron Diffraction Studies on Residual Stress Behavior in Powder Bed Fusion Metals
A.S. Wu*, **G.F. Gallegos**, **M. Kumar**, **M.W. Wraith**, **S.C. Burke**, Lawrence Livermore National Laboratory, Livermore, CA, USA
D.W. Brown, Los Alamos National Laboratory, Los Alamos, NM, USA

9:00 **D-15** High Energy Synchrotron X-ray Diffraction Measurements of Simple Bending of Pseudoelastic NiTi Shape Memory Wires
B. Zhang*, **M.L. Young**, University of North Texas, Denton, TX, USA

9:20 **D-33** Effect of Granular Constraints on Phase Transformation in Shape Memory Alloys – A Coupled Synchrotron X-ray Diffraction and Micromechanical Modeling Study
H.M. Paranjape*, Colorado School of Mines, Golden, CO, USA and Northwestern University, Evanston, IL, USA
A.P. Stebner, Colorado School of Mines, Golden, CO, USA
J.-S. Park, **H. Sharma**, APS - Argonne National Laboratory, Argonne, IL, USA
L.C. Brinson, Northwestern University, Evanston, IL, USA

9:40 **D-49** In-Situ Characterization of Piezoelectric Materials via X-ray Diffraction
J. Giencke*, **B. Jones**, Bruker AXS, Madison, WI, USA

10:00 **D-24** Leveraging New Technologies for Stress Analysis of Complex Shapes with a Laboratory Diffractometer
A. Adibhatla*, **S. Speakman**, PANalytical, Inc., Westborough, MA, USA

10:20 **Break**

10:40 **F-50** Micro- and Nano Scale *in situ* X-ray CT as a Diagnostic for Material Performance
B.M. Patterson*, **A. Clarke**, **S. Imhoff**, **R. Pacheco**, **E. Weis**, **K. Henderson**, **N. Cordes**, Los Alamos National Laboratory, Los Alamos, NM, USA
B. Hornberger, Carl Zeiss X-ray Microscopy Inc.

11:00 **D-32** Invited - MAUI: Modeling, Analysis and Ultrafast Coherent Imaging
R. Harder*, **T. Peterka**, **I. McNulty**, **H. Wen**, **S. Sankaranarayanan**, **S. Leyffer**, **T. Munson**, **N. Ferrier**, Argonne National Laboratory, Argonne, IL, USA

11:30 **D-47** Invited - High-resolution Biological Cryo-ptychography
D.J. Vine*, Argonne National Lab, Argonne, IL, USA

Applied Materials — Standley II

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

8:30 **D-57** Invited - Pharmaceutical Materials Science – Unique Role of XRD in the Characterization and Quantification of Crystalline Phases
R. Suryanarayanan*, University of Minnesota, Minneapolis, MN, USA

9:00 **D-16** Single-crystal X-rays Structure Analysis of One Drug Powder by the Spring-8 Synchrotron Radiation X-ray
T. Hashimoto*, **S. Honda**, **N. Yasuda**, **S. Kimura**, JASRI/Spring-8, Hyogo, Japan
S. Hayakawa, JASRI/Spring-8, Hyogo, Japan and Hiroshima University, Hiroshima, Japan
Y. Nishiwaki, JASRI/Spring-8, Hyogo, Japan and Kochi University, Kochi, Japan
M. Takata, JASRI/Spring-8, Hyogo, Japan and University of Tokyo, Tokyo, Japan

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9:20	**D-27**	X-ray Study of Amorphous Scattering of Atactic Polystyrene Films **Y. Tang**, **J. Yin**, **L.-Z. Liu***, Sinopec Beijing Research Institute of Chemical Industry, Beijing, China
9:40	**D-35**	Elucidation of Sequence-Dependent Structure/Function Relationships for Bio-Enabled Nanoparticles **N.M. Bedford***, National Institute of Standards and Technology, Boulder, CO, USA
10:00	**D-38**	X-ray Investigations of Solid Solutions and Phase Transitions of Monocalciumaluminate and Monobariumaluminate Use in Cement, Phosphorescence and Radiation Protection Applications **H. Pöllmann***, **R. Kaden**, University of Halle, Saale, Germany
10:20		**Break**
10:40		Invited - Title to be Announced **B.G. Landes**, Dow Chemical Company, Midland, MI, USA
11:10	**D-8**	Role of Element Partitioning on the α - ß Phase Transformation Kinetics of a bi-modal Ti-6Al-6V-2Sn Alloy during Continuous Heating **P. Barriobero-Vila***, Vienna University of Technology, Vienna, Austria **G. Requena**, German Aerospace Center (DLR), Cologne, Germany and Institute of Metal Forming, RWTH Aachen University, Aachen, Germany **T. Buslaps**, ESRF, Grenoble, France **M. Alfeld**, **U. Boesenberg**, DESY, Hamburg, Germany
11:30	**D-23**	Unidirectional Thermal Expansion in Edge-sharing BO_4 Tetrahedra Contained $KZnB_3O_6$ **Y. Lou**, **D. Li**, **Z. Li**, **S. Jin***, **X. Chen**, Institute of Physics - Chinese Academy of Sciences, Beijing, China
11:50	**D-18**	Ferroelectric Domains in Strained (K,Na)NbO_3 Epitaxial Thin Films on (110)$TbScO_3$ Substrate Studied by X-ray Diffraction **M. Schmidbauer***, **A. Kwasniewski**, **D. Braun**, **J. Sellmann**, **P. Müller**, **J. Schwarzkopf**, Leibniz-Institute for Crystal Growth, Berlin, Germany **M. Hanke**, Paul-Drude Institut für Festkörperelektronik, Berlin, Germany

General XRF — Cotton Creek

Chair: **U.E.A. Fittschen**, Washington State University, Pullman, WA, ursula.fittschen@wsu.edu

9:00	**S-18**	Invited - Understanding Material Structure and Performance with 3D X-ray Imaging **B.M. Patterson***, **A. Ionita**, **D. Dalvit**, **D.S. Moore**, **K. Henderson**, **N. Cordes**, Los Alamos National Laboratory, Los Alamos, NM, USA **N. Chawla**, **A.R. Ovejero**, **T. Stannard**, **S. Singh**, Arizona State University, Tempe, AZ, USA **X. Xiao**, Argonne National Laboratory, Argonne, IL, USA
9:30	**F-15**	Thin Film XRF Specimen Preparation: Improvements over the Dried Spot Approach **C.G. Worley***, Los Alamos National Laboratory, Los Alamos, NM, USA
9:50	**F-3**	Characterization of Flat and Curved Pyrolytic Graphite Mosaic Crystals **Y. Van Haarlem***, CSIRO, Sydney, NSW, Australia **J. Tickner**, CSIRO, Adelaide, SA, Australia
10:10		**Break**
10:40	**F-57**	Invited - A Bright Future without High X-ray Brilliance: Applications of Modern Laboratory-Based XAFS and XES **G.T. Seidler***, **D. Mortensen**, **A. Ditter**, **N. Ball**, **A. Remesnik**, University of Washington, Seattle, WA, USA
11:10	**F-2**	Development and Performance of Microfluidic Flow-based Sample Introduction for Direct Analysis of Liquids by Micro X-ray Fluorescence Spectrometry **K.G. McIntosh***, **G.J. Havrilla**, Los Alamos National Laboratory, Los Alamos, NM, USA
11:30	**F-29**	BIO MASS: Waste or Valuable - In Any Case the Analytical Solution is XRF **F. Portala**, **K. Behrens***, **A. Wegner**, **J. Stelling**, Bruker AXS, Karlsruhe, Germany **D. Pecard**, **A. Buman**, Bruker AXS, Madison, WI, USA
11:50	**F-37**	Uncertainties and Discriminators in X-ray Spectroscopy **T. Papp**, **J.A. Maxwell**, Cambridge Scientific, Ontario, Canada

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Oral Sessions – Thursday Afternoon

**Signifies Presenting Author, when noted*

Energy Materials — Standley I

Chair: **M.A. Rodriguez**, Sandia National Laboratory, Albuquerque, NM, marodri@sandia.gov

1:30 **S-22** Invited - Probing Energy Materials with High Energy X-rays
K. Chapman, APS - Argonne National Laboratory, Argonne, IL, USA

2:00 **S-23** Invited - X ray and Neutron Scattering to Characterize Oxide Nanosheets for Supercapacitor Electrodes
P. Metz*, **B. Cladek**, **T. Hey**, **P. Gao**, **D. Liu**, **S.T. Misture**, Alfred University, Alfred, NY, USA
J. Neuefeind, **K. Page**, Oak Ridge National Lab, Oak Ridge, TN, USA
R. Koch, University of Trento, Trento, Italy

2:30 **S-4** New Insights into OER Active Noble Metal Surfaces - *In situ* GIXRD and XRR Measurements in Electrochemical Catalysis
M. Scherzer, **F. Girgsdies**, **M. Friedrich**, **E. Frei**, **R. Schlögl**, Fritz Haber Institut der MPG, Berlin, Germany

2:50 **D-20** X-ray Nanodiffraction Study of the Delithiation Mechanism of $LiFePO_4$ Single Particles
B. May*, **J. Cabana**, University of Illinois-Chicago, Chicago, IL, USA
Y. Yu, Lawrence-Berkeley National Laboratory, Berkeley, CA, USA and University of Illinois-Chicago, Chicago, Illinois, U.S.A.
M.V. Holt, Argonne National Laboratory, Argonne, IL, USA
F. Strobridge, **C.P. Grey**, University of Cambridge, Cambridge, UK

3:10 **Break**

3:30 **S28** Invited - Using Neutron Reflectometry to Investigate Solid-Electrolyte Interphase Formation, *in situ*, in Li Ion Battery Materials
J. Browning*, **G.M. Veith**, **M. Doucet**, Oak Ridge National Laboratory, Oak Ridge, TN, USA

4:00 **D-56** Using Energy Dispersive X-ray Diffraction to Map Li-Ion Batteries
J.S. Okasinski*, **D. Abraham**, Argonne National Laboratory, Argonne, IL, USA

4:20 **S-3** Analytical Imaging of Batteries with X-ray Compton Scattering
Y. Sakurai*, **M. Itou**, **M. Brancewicz**, JASRI, Sayo, Japan
H. Sakurai, **K. Suzuki**, Gunma University, Gunma, Japan
Y. Orikasa, **Y. Uchimoto**, Kyoto University, Kyoto, Japan

4:40 **D-43** Investigation through XRD Techniques of Advanced Materials for High Temperature Power Plant Applications
E. Barbareschi*, **A. Costa**, **E. Vacchieri**, Ansaldo Sviluppo Energia SpA, Genova, Italy

General XRD — Standley II

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

1:30 **D-17** Invited - Application of Patterson-function Direct Methods and Synchrotron *tts*-microdiffraction to Structural Studies of Intermediate Phases of Zeolites: The Laumontite and Ilerdite Case
J. Rius*, **A. Crespi**, **C. Frontera**, Institut de Ciència de Materials de Barcelona (CSIC), Catalonia, Spain
O. Vallcorba, ALBA Synchrotron Facility-CELLS, Catalonia, Spain

2:00 **D-11** Novel XRD Methods for Handheld Instrumentation
G.M. Hansford*, University of Leicester, Leicester, UK

2:20 **D-14** Synchrotron X-ray Diffraction Mapping of a Friction Stir-processed $Al_{0.1}CoCrFeNi$ HEA
N.A. Ley*, **M. Komarasamy**, **R. Mishra**, **M.L. Young**, University of North Texas, Denton, TX, USA

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2:40 **D-30** Powder Diffraction Experiments at the ID11 Beamline (ESRF, Grenoble)
A. Bernasconi*, **J. Wright**, **N. Harker**, **H. Gleyzolle**, **M. Ruat**, ESRF, Grenoble, France
M. Coduri, National Centre of Research, Institute for Energetics and Interphases – Lecco, Italy

3:00 **Break**

3:30 **D-51** Study of SRM 660B Using Neutron Time-Of-Flight Diffraction Data from Powgen at the Spallation Neutron Source (SNS)
J. Faber, Faber Consulting, Thornton, PA, USA
P. Whitfield, **E.A. Payzant**, Oak Ridge National Laboratory, Oak Ridge, TN, USA

3:50 **D-53** Characterization of the Cu Kα Emission Spectrum
J.P. Cline, **M. Mendenhall**, **D. Windover**, **A. Henins**, NIST, Gaithersburg, MD, USA

4:10 **D-10** Fast Synthesis and Refinement of the Atomic Pair Distribution Function
A.A. Coelho, Brisbane, Australia
P.A. Chater, Diamond Light Source, Didcot, Oxfordshire, UK
A. Kern*, Bruker AXS GmbH, Karlsruhe, Germany

4:30 **S-20** The Use of Atomic Pair Distribution Function (PDF) and X-ray Scattering Methods to Assess the Stability of Amorphous and Nanocrystalline Organic Compounds: A Comparative Study of Synchrotron Radiation and a Laboratory Diffractometer
A. Adibhatla*, PANalytical Inc, Westborough, MA, USA
D. Beckers, **M. Gateshki**, PANalytical B.V., Almelo, The Netherlands
H. Novoa de Armas, Johnson and Johnson Pharmaceutical R&D, Beerse, Belgium

4:50 **D-19** Data Evaluation Algorithms for Two-Dimensional XRD
B.B. He, Bruker AXS, Madison, WI, USA

Environmental & Geological Applications — Cotton Creek

Chairs: **R. Van Grieken**, University of Antwerp, Antwerp, Belgium, rene.vangrieken@uantwerpen.be
J. Miranda, Universidad Nacional Autónoma de México, México, miranda@fisica.unam.mx

2:00 **F-1** Invited - Characterization of Particulate Air Pollution in Kingston, Jamaica
J. Boman*, **S.M. Gaita**, University of Gothenburg, Gothenburg, Sweden

2:30 **F-59** Invited - PIXE as a Screening Technique for Consumer Products
G.F. Peaslee*, **L.R. Savagian**, **A.M. Maley**, **E.E. Greve**, **S. Dorn**, **P.A. DeYoung**, Hope College, Holland, MI, USA

3:00 **F-5** A New Device for the Simultaneous Application of PIXE and XRF in Vacuum
J. Miranda*, **J. Reyes-Herrera**, **O.G. de Lucio**, Universidad Nacional Autónoma de México, México

3:20 **Break**

3:50 **F-41** Geographical Profiling and Sand Analysis: What Information We Can Extract from Compositional Pattern of Sands
S. Mamedov*, Horiba Scientific, Edison, NJ, USA

4:10 **F-27** The Application of SumXcore Technology to Improve the Analysis of Geological Materials
A. Komelkov*, **Y. Xiao**, **C. Tsouris**, PANalytical B.V., Almelo, The Netherlands

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Oral Sessions – Friday Morning

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Rietveld **Standley I**

Chair: **S. Antao**, University of Calgary, Calgary, AB, Canada, antao@ucalgary.ca

8:00 **D-1** Invited - The Effect of High Pressure and Disorder on Negative Thermal Expansion Materials Examined by Powder Diffraction
A.P. Wilkinson*, Georgia Institute of Technology, Atlanta, GA, USA

8:30 **D-4** Vibrational Spectroscopy Study of $Ba_{2-x}Sr_xMgMoO_6$
R. Abkar*, **B. Manoun**, **A. Hachimi**, **A. Elaamrani**, Université Hassan 1er, Morocco
S. Benmokhtar, LRCPGM, Faculté des Sciences Ben M'Sik Casablanca, Maroc
P. Lazor, Uppsala University, Uppsala, Sweden

8:50 **D-41** Pyrope-majorite Solid Solutions: Is there a Phase Transition?
S.M. Antao*, **N.S. Suarez Nieto**, University of Calgary, Calgary, AB, Canada
G.D. Gwanmesia, Delaware State University, Dover, DE, USA

9:10 **D-52** Invited - Successes and Challenges of High Pressure Neutron Powder Diffraction
A.M. dos Santos*, **C.A Tulk**, **J.J. Molaison**, Oak Ridge National Laboratory, Oak Ridge, TN, USA
M. Guthrie, European Spallation Source, Lund, Sweden

9:40 **D-28** Total Scattering Measurements and Modeling in Aluminosilicate-based Glasses
A. Bernasconi*, ESRF, Grenoble, France

10:00 **Break**

10:20 **S-2** Invited - X-ray Diffraction and Beyond: Quantification and Evaluation of Crystalline and Amorphous Phases in Cements
J. Anderson*, PANalytical, Montreal, QC, Canada
T. Füllmann, **T. Witzke**, PANalytical B.V., Almelo, The Netherlands

10:50 **D-12** Amorphous Quantification of *in-situ* XRPD Data using the K-Factor Approach
S.A. Speakman, **A. Adibhatla**, PANalytical, Westborough, MA, USA
T. Degen, PANalytical B.V., Almelo, The Netherlands

11:10 **D-26** Invited - Application of Powder X-ray Diffraction Technique in Drug Discovery & Development
H. Park, Bristol-Myers Squibb, Wallingford, CT, USA

11:40 D-9 Synthesis, Investigation on the Crystal Structure by Rietveld Refinement of the Double Perovskite $Ba_{0,4}Sr_{1,6}NiMoO_6$
A. EL Aamrani*, **B. Manoun**, **R. Abkar**, **Y. Tamraoui**, **F. Mirinioui**, Université Hassane Ier, Morocco
S. Benmokhtar, LRCPGM, Faculté des Sciences Ben M'Sik Casablanca, Maroc
P. Lazor, Uppsala University, Uppsala, Sweden

Micro XRF **Standley II**

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

8:30 **F-45** Invited - Confocal Micro-XRF Analysis for Monitoring Chemical Reactions
K. Tsuji*, **J. Chin**, **M. Yamanashi**, **Y. Kitado**, Osaka City University, Osaka, Japan

9:00 **F-33** Micro X-ray Fluorescence: Instrumentation and Applications
G.J. Havrilla*, **K. McIntosh**, **V. Lopez**, Los Alamos National Laboratory, Los Alamos, NM USA

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9:20 **F-16** An Overview of the Mars 2020 Mission Micro-XRF Instrument PIXL
L.A. Wade*, **A. Allwood**, **M. Foote**, **D. Dawson**, **E. Ek**, **C. Liebe**, **B. Hernandez**, **R. Sharrow**, California Institute of Technology, Pasadena, CA, USA
S. Battel, Battel Engineering, Scottsdale, AZ, USA
M. Panning, University of Michigan, Ann Arbor, MI, USA
K. Kozaczek, **T. Parker**, Moxtek Inc., Orem, UT, USA
N. Gao, XOS, Greenbush, NY, USA
A. Huber, Amptek, Bedford, MA, USA
J. Hurowitz, Stony Brook University, Stony Brook, NY, USA
E. Hertzberg, Hertzberg Engineering, Mountain View, CA, USA

9:40 **Break**

10:00 **F-56** Invited Tuning the 'lens' of X-ray Fluorescence Imaging: In Pursuit of Chemical Speciation
L. Finney*, APS, Argonne National Laboratory, Lemont, IL, USA

10:30 **F-42** MicroXRF Analysis of Astrobiologically-Significant Geological Samples
D.T. Flannery*, Caltech/NASA Jet Propulsion Laboratory, Pasadena, CA, USA
A.C. Allwood, **R. Hodyss**, **D.R. Thompson**, **L. Wade**, NASA Jet Propulsion Laboratory, Pasadena, CA, USA
W.T. Elam, University of Washington, Seattle, WA, USA

10:50 **F-49** Discriminating Glass Fragments Using Micro-XRF Spectrometry with Poly-capillary Optics
B. Scruggs, EDAX Mahwah, NJ, USA

Fusion & Industrial Applications of XRF — Cotton Creek

Chairs: **J. Anzelmo**, Anzelmo & Associates, Inc., Madison, WI, jaanzelmo@aol.com
M. van der Haar, PANalytical, Westborough, MA, marco.van.der.haar@panalytical.com

8:30 **F-36** Invited - Rapid Quantitative Analysis of Solids by X-ray Fluorescence Spectroscopy Using Sample Fusion and the Standard Additions Method
D.B. Aeschliman*, **J.A. Bender**, 3M Company, Saint Paul, MN, USA

9:00 **F-30** X-ray Fluorescence has Multiple Layers - At-Line, On-Line & In-Line
F. Portala, **K. Behrens**, **A. Wegner**, **J. Stelling**, Bruker AXS, Karlsruhe, Germany
A. Buman, **D. Pecard**, Bruker AXS, Madison, WI, USA

9:20 **F-26** Process Control Made Easy - Which Technology Do You Prefer
F. Portala, **K. Behrens**, Bruker AXS, Karlsruhe, Germany
D. Pecard, **A. Buman**, Bruker AXS, Madison, WI, USA

9:40 **F-25** The Benefits of Small Spot Mapping Analysis in Production Process Troubleshooting using an XRF Spectrometer Containing WD and ED Cores
F. Casco-Tañeza, PANalytical BV, Almelo, The Netherlands

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2015 Denver X-ray Conference and TXRF 2015 ♦ 3 – 7 August, Westin, Westminster, CO
Program-at-a-Glance

Monday Morning Workshops ♦ 9:00 am – 12:00 Noon					
	Standley I	Standley II	Cotton Creek	Meadowbrook	Lake House
XRD	Basic to Advanced XRD I (**Misture/Blanton/Fawcett**)	Structure Determination from Laboratory XRPD Data (**Kern/Madsen**)			
XRF			Basic XRF (**Drews**)		
Monday Afternoon Workshops ♦ 1:30 – 4:30 pm					
XRD	Basic to Advanced XRD II (**Misture/Blanton/Fawcett**)	Fundamentals of Neutron Diffraction (**Whitfield**)			
XRF			Energy Dispersive XRF (**Phillips**)	Micro XRF (**Havrilla**)	
Monday Evening XRD Poster Session & Reception 5:00 – 7:00 pm. Westminster Foyer (Watkins)					
Tuesday Morning Workshops ♦9:00 am – 12:00 Noon					
XRD	Stress (**Noyan**)	Quantifying Crystalline & Amorphous Phases I (**Kern/Madsen**)			
XRF			Quantitative Analysis I (**Mantler**)	Uncertainty in XRF (**Kawai**)	
TXRF2015					Introduction to TXRF (**Wobrauschek/Streli**)
Tuesday Afternoon Workshops ♦ 1:30 – 4:30 pm					
XRD	Synchrotron X-ray Coherent Diffraction Imaging and Ptychography (**Holt**)	Quantifying Crystalline & Amorphous Phases II (**Kern/Madsen**)			
XRF			Quantitative Analysis II (**Mantler**)	Sample Preparation of XRF (**Anzelmo**)	
TXRF2015					TXRF Standardization (**Tsuji**)
Tuesday Evening XRF & TXRF Poster Session & Reception 5:00 pm – 7:00 pm. Westminster Foyer (Broton/Anzelmo)					
Wednesday Morning Plenary Session, TXRF Around The World (**Zaitz**).8:30 – 11:45. Standley Ballroom					
Wednesday Afternoon Sessions					
Special Topics	New Developments in XRD/XRF Instrumentation (**Blanton/Fawcett**)	Extremely Bright: The Future of X-ray Analysis (**Vogt/Murray**)			
XRF			Quantitative Analysis (**Brehm**)		
TXRF2015				TXRF General Session	
Wednesday Evening Vendor Sponsored Reception 5:30 pm – 7:00 pm. Exhibit Hall/Westminster Ballroom					
Thursday Morning Sessions					
XRD	Stress Analysis/Ptychography (**Watkins/Holt**)	Applied Materials (**Fawcett/Blanton**)			
XRF			General XRF (**Fittschen**)		
TXRF2015				TXRF Environmental	
Thursday Afternoon Sessions					
Special Topics	Energy Materials (**Rodriguez**)				
XRD		General XRD (**Murray**)			
XRF			Environmental & Geological (**van Grieken/Miranda**)		
TXRF2015				TXRF Biological SR-TXRF	
Friday Morning Sessions					
XRD	Rietveld (**Antao**)				
XRF		Micro XRF (**Havrilla**)	Fusion & Industrial Apps (**Anzelmo/van der Haar**)		
TXRF2015				TXRF Semiconductor	

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- Similarity indexes — their use and value
- How to choose coordinate structures for Rietveld Refinement

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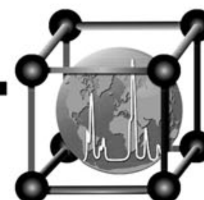

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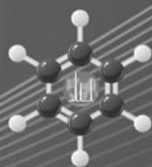

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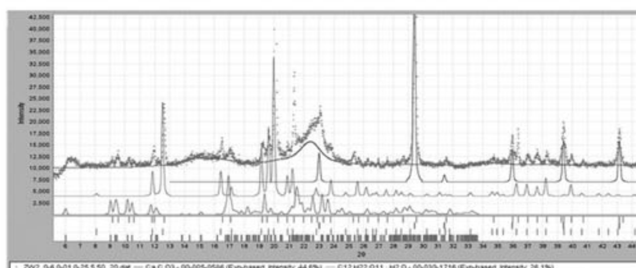

The four phase identification of the formulation of Lipitor uses references from a single crystal determination, an experimental powder pattern of cellulose Iβ, a calculated powder pattern and pattern extracted from the patent literature. The identification required an inorganic excipient, polymer excipient and two organic compounds. A variety of reference materials and sources enabled the identification.

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Professor Bogdan Lazoryak

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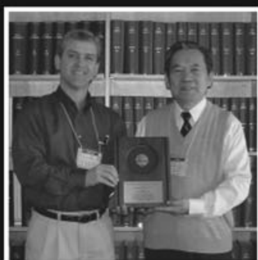
presenting to
Dr. Sergei Kirik

2004: (R)
Dr. Tom Blanton
presenting to
Professor Shao-Fan Lin



2001: (L)
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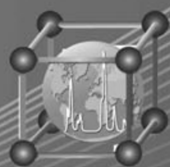

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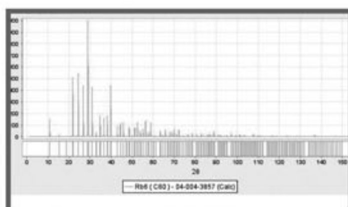

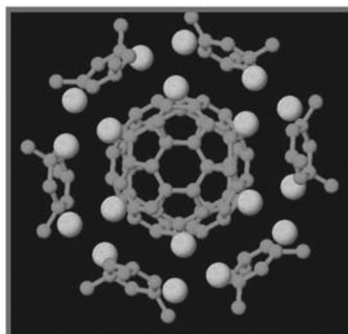

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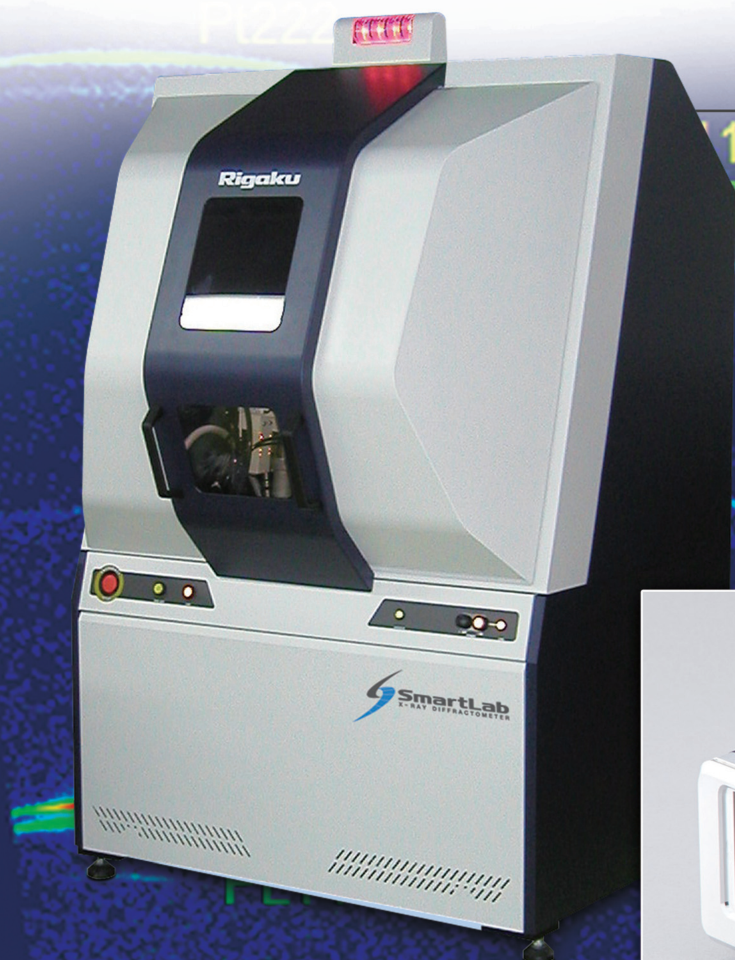

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