INTERNATIONAL CENTRE FOR DIFFRACTION DATA

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DENVER X-RAY CONFERENCE
67th Annual Conference on Applications of X-ray Analysis

6 - 10 August 2018 • The Westin, Westminster, Colorado, USA

2018 Program

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The information contained in this PDF is current as of April 2018. Updates to the Program can be viewed on the Program page of the Denver X-ray Conference website:

www.dxcicdd.com

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DENVER X-RAY CONFERENCE ORGANIZING COMMITTEE

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Randy Barton, USA

Victor Buhrke, USA

W. Tim Elam, University of Washington APL, USA

George Havrilla, Los Alamos National Laboratory, USA

Clay Ruud, USA

Future Conference:

DENVER X-RAY CONFERENCE®
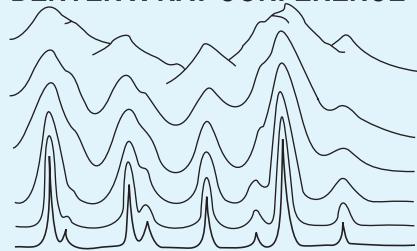
5-9 August 2019
The Westin Lombard Yorktown Center, Lombard, IL, USA

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Poster Sessions

Oral Sessions

Exhibit Hours and Participating Companies as of April 2018
Exhibits will be held in the Westminster Ballroom.

Exhibit Hours

Tuesday, 7 August:	10:00am - 5:00pm
Wednesday, 8 August:	12:00pm - 7:00pm
Thursday, 9 August:	10:00am - 2:00pm

Participating Companies

AMPTEK, Inc.
Angstrom, Inc.
Anton Paar
ASI
ASI Standards
AXO DRESDEN/Huber Diffraction Equipment
Brightspec NV/SA
Bruker
Chemplex Industries, Inc.
DECTRIS, Ltd.
Excillum
G.N.R.S.R.L.
Heraeus
Herzog Automation Corp.

Hitachi High-Tech Science America, Inc.
Inrad Optics
International Centre for Diffraction Data
IXRF Systems, Inc.
KETEK GmbH
Malvern Panalytical
Materials Data, Inc.
Materion Electrofusion
Micro X-Ray, Inc.
Micromatter Technologies, Inc.
MOXTEK, Inc.
PNDetector GmbH
PREMIER Lab Supply, Inc.
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RaySpec, Ltd.
Rigaku Americas
Shimadzu Scientific Instruments, Inc.
Specac Limited
SPECTRO Analytical Instruments
SPEX SamplePrep/Katanax
STOE & Cie GmbH
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Thermo Fisher Scientific
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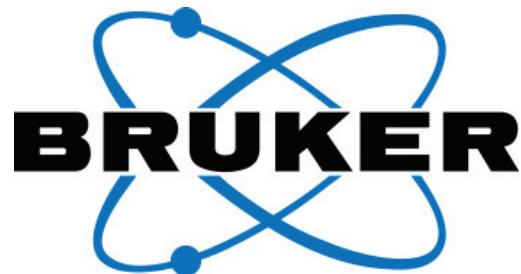
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Monday Morning Workshops 9:00 am – 12:00 Noon

Material Identification – The good, bad and ugly   Standley I
Organizers & Instructors:
T. Fawcett, Emeritus ICDD, USA, dxcfawcett@outlook.com
J. Blanton, S. Kabekkodu, ICDD, USA, jblanton@icdd.com; kabekkodu@icdd.com

All automated search match algorithms and applications are based on sound fundamental assumptions about how the specimen is prepared, and the influence of several instrumental parameters used in your experiment. However, in practice, there are numerous cases where these assumptions are not met, many times for perfectly good reasons, leading to inaccuracies and false identifications. We will use dozens of case histories to show how various problems can be identified with practical solutions to these problems.

Selecting Software for Rietveld Refinement I   Lake House
Organizer & Instructors
A.A. Yakovenko, L.C. Gallington, Argonne National Laboratory, USA, ayakovenko@anl.gov; gallington@anl.gov
A.F.M. Dos Santos, Oak Ridge National Laboratory, USA, dossantosam@ornl.gov
S.N. Rodesney, Bruker AXS, Inc., USA, steven.rodesney@bruker.com

Introduction to the Structure Determination and Structure Analysis from Powder Diffraction often starts with the selection of Rietveld refinement software. Different groups are usually selecting software for several reasons. One of the major reasons, is that such particular software is better suited and have tools which allow "simple" process of powder diffraction data from the materials which are being studied, or from instrument where this data have been collected. However, for a person who has just been introduced to the Powder Diffraction Science, such diversity of the software might be confusing. Very often students and early career scientists do not know where to start, and which software to use for their particular problems.

The 2018 Rietveld Refinement workshop will show a variety of Rietveld refinement software, highlighting the tools, methods which are suited for particular types of refinement and/or classes of materials. This would allow students to choose the software for their need or discover new functions and routes of refinements.

Basic XRF   Standley II
Organizer & Instructors:
J.A. Anzelmo, Anzelmo & Associates, Inc., USA, jaanzelmo@aol.com
M.A. Zaitz, IBM, USA, zaitz@us.ibm.com

This workshop provides a basic introduction to the principles of XRF and is specifically aimed at those new to the field. It begins with a general overview of the technique and the various instrumentation configurations including their main applications. This is followed by more specific details of XRF Physics. Basic WDX instrumentation will be described with its use and applications. In the second half of the workshop, basic EDX instrumentation including general purpose bulk analyzers (benchtop EDX), TXRF, Micro analyzers, and Handheld analyzers will be reviewed. Capabilities and applications in actual practice will be described.

Quantitative Analysis of XRF I   Cotton Creek
Organizer & Instructors:
W.T. Elam, University of Washington, USA, wtelam@apl.washington.edu
B. Vrebos, Malvern PANalytical, The Netherlands, bruno.vrebos@panalytical.com
K. Kawakyu, Rigaku Corporation, Japan, kawakyu@rigaku.co.jp

Part I: Matrix effects and how to compensate for them: scatter peaks, compensation methods, semi-quantitative analysis using FP, and fusion.

Part II: Walkthrough of quantitative analysis for a few XRF spectra.

Monday Afternoon Workshops 1:30 pm – 4:30 pm

Quantitative Phase Analysis
Standley I

<u>Organizer</u> & Instructors:
E. Ryba, Penn State University, USA, rx7@psu.edu
J. Kaduk, Poly Crystallography, Inc. and Illinois Institute of Technology, USA, kaduk@polycrystallography.com
N. Henderson, Bruker AXS, Inc., USA, nathan.henderson@bruker.com

This workshop on X-ray diffraction methods for quantitative phase analyses begins with a series of examples of manual single-peak analyses using standards and reference intensity ratios. An introduction to full-pattern methods is next, followed by discussions of things that can go wrong (e. g., instrument aberrations, absorption, surface roughness, microabsorption, preferred orientation) and the accuracy attainable. The approaches for the quantification of amorphous content will be addressed, including the use of calibration curves, internal standards, total integrated intensities, and the 'Partial or No Known Crystal Structure' method. Interesting examples for a wide variety of materials throughout.

Two-Dimensional Detectors
Standley II

<u>Organizers</u> & Instructors:
T.N. Blanton, ICDD, USA, tblanton@icdd.com
B.B. He, Bruker AXS, Inc., USA, bob.he@bruker.com
M. Mueller, DECTRIS, Switzerland, marcus.mueller@dectris.com
J. Ferrara, Rigaku, USA, Joseph.Ferrara@rigaku.com
S. Speakman, Malvern PANalytical, USA, scott.speakman@panalytical.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.

Selecting Software for Rietveld Refinement II
Lake House

<u>Organizer</u> & Instructors:
A.A. Yakovenko, L.C. Gallington, Argonne National Laboratory, USA, ayakovenko@anl.gov; gallington@anl.gov
A.F.M. Dos Santos, Oak Ridge National Laboratory, USA, dossantosam@ornl.gov
S.N. Rodesney, Bruker AXS, Inc., USA, steven.rodesney@bruker.com

Continuation from the morning workshop, Selecting Software for Rietveld Refinement I (see description on page 2).

Quantitative Analysis of XRF II
Cotton Creek

<u>Organizer</u> & Instructors:
W.T. Elam, University of Washington, USA, wtelam@apl.washington.edu
B. Vrebos, Malvern PANalytical, The Netherlands, bruno.vrebos@panalytical.com
K. Kawakyu, Rigaku Corporation, Japan, kawakyu@rigaku.co.jp

Continuation from the morning workshop, Quantitative Analysis of XRF I (see description on page 2).

Energy Dispersive XRF
Meadowbrook

<u>Organizer</u> & Instructors:
P. Lemberge, Thermo Fisher Scientific, Switzerland, pascal.lemberge@thermofisher.com
W.D. Watson, Thermo Fisher Scientific, USA, wayne.watson@thermofisher.com
V. Osorio, Brightspec NV/SA, Belgium, vicente.osorio@brightspec.be

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; spectrum fitting; rapid qualitative analysis; 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.

Tuesday Morning Workshops 9:00 am – 12:00 Noon

Characterization of Thin Films   Standley I

Organizer & Instructors:

K. Hradil, W. Artner, TU Wien, Austria, klaudia.hradil@tuwien.ac.at; werner.artner@tuwien.ac.at

The workshop will include the theoretical background and experimental techniques of thin film analysis by X-ray diffraction methods. This will include the experimental techniques and the analysis of data for grazing incidence diffraction and reflectivity investigations and also high resolution methods. The possibilities for the microstructure properties analysis of thin films like stress/strain and texture analysis, classical phase analysis and thin film crystallinity properties with lab methods will be introduced for selected examples. Furthermore, we will discuss measurement techniques for beam sizes in the micro- (lab) and nano-scale (synchrotron).

Line Profile Analysis   Standley II

Organizer & Instructors:

M. Leoni, University of Trento, Italy, matteo.leoni@unitn.it

J. Cline, M. Mendenhall, NIST, USA, james.cline@nist.gov; marcus.mendenhall@nist.gov

L. Sweet, PNNL, USA, lucas.sweet@pnnl.gov

The determination of microstructure parameters (such as size of the domains or type and quantity of lattice defects) is still one of the most frequent applications of powder diffraction. In the last 100 years we moved from single peak to full pattern analysis and from qualitative to quantitative results. Several standards have been specifically developed by the NIST to address the issues of characterizing the instrumental contribution and validating the analysis techniques. An historical overview of the available techniques and assessment of the state of the art will be made, providing some practical examples of application and advices on the meaning of the results. BYOD (Bring Your Own Data) for a more active discussion!

Micro XRF   Cotton Creek

Organizer & Instructors:

M.A. Zaitz, IBM, USA, zaitz@us.ibm.com

N. Gao, XOS, USA, ngao@xos.com

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

Micro XRF analysis has become an integral part of the lab analysis and is used in a wide variety of fields, such as: art and archeology, bioengineering, semiconductor, environmental, criminal forensics or industrial quality control work. The strength of micro XRF is multi element energy dispersive XRF analysis which is relatively fast analysis, may require little or no sample prep, and combined with elemental mapping provides another depth of information. The Micro XRF workshop will provide an overview of micro X-ray fluorescence (MXRF) including brief review of the basics of ED-XRF analysis, a status of current instrumentation, an introduction of the physics of capillary optics and a current state of the art micro optic systems. Various types of applications including qualitative and quantitative with calibration options such as basic empirical, standardless FP and semiquant FP. The workshop will explore elemental imaging (mapping/scanning) as well as their particularities. An update on 3D confocal micro XRF analysis will be presented.

Sample Preparation of XRF   Meadowbrook

Organizer & Instructors:

J.A. Anzelmo, Anzelmo & Associates, Inc., USA, jaanzelmo@aol.com

C. Audet, Claisse, Canada, caudet@claisse.com

This workshop will focus more on the different aspects of fusion for both simple and difficult samples. It will begin with borate fusion preparation, but for the first time in this workshop, we will also discuss the chemistry of peroxide fusions and its applications. The Physics of XRF sample preparation will also be discussed as usual, as well as pressed powder preparation. These techniques and methods are essential in today's modern laboratory.

Tuesday Afternoon Workshops 1:30 pm – 4:30 pm

Imaging   Standley I

Organizer & Instructors:

S. Vogt, Argonne National Laboratory, USA, svogt@anl.gov

Instructors to be announced.

X-ray imaging and microscopy as had tremendous impact over the past decade, addressing extremely broad and highly relevant scientific and industrial questions. It is particularly well suited to visualizing materials across numerous lengthscales, in depth, and in situ/operando. Application areas are as broad as high-speed imaging of laser fusion processes in additive manufacturing, mapping trace elements in biological systems to better understand their impact on human health both in their natural occurrence and via therapeutic drugs, or nanoscale imaging of integrated circuitry with the goal of process verification and failure analysis. We will discuss methods and techniques in areas of full-field imaging, tomography, scanning probe techniques, as well as lensless imaging approaches. In addition to instrumentation related topics, we will discuss computational approaches.

Non-Ambient   Standley II

Organizer & Instructors:

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

E.A. Payzant, Oak Ridge National Laboratory, USA, payzanta@ornl.gov

A. Jones, Anton Paar GmbH, Austria, andrew.jones@anton-paar.com

H. zur Loye, University of South Carolina, USA, zurloye@mailbox.sc.edu

This half-day workshop will focus on high temperature XRD in laboratory instruments and will include an overview of the capabilities of the various commercially-available non-ambient stages. Pitfalls, tips and tricks for using non-ambient stages for controlled temperature, gaseous atmosphere, and applied electric fields will be covered with brief examples. Topics will include temperature calibration, accuracy of the XRD patterns (instrument optics, calibration and/or corrections for specimen displacement) and handling the resulting large datasets to obtain phase ID, cluster analysis, and (automated) Rietveld full-pattern fitting.

Trace Analysis   Cotton Creek

Organizers & Instructors:

C. Streli, P. Wobrauschek, TU Wien, Atominstitut, Austria, streli@ati.ac.at; wobi@ati.ac.at

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

N. Kawahara, Rigaku, Japan, kawahara@rigaku.co.jp

Both beginners and experienced X-ray scientists and applicants, physicists and chemists, should gain information by attending the Trace Analysis Workshop. Presentations of most modern techniques and instrumentation for trace element analysis using EDXRS and 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 μ-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 importance 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.

Handheld XRF – The Silver Bullet or Fools Gold?   Meadowbrook

M. Loubser, GeoMagGeoChem, South Africa, maggi.loubser@gmail.com

A. Seyfarth, SGS North America, Canada, alexander.seyfarth@sgs.com

X-ray fluorescence spectroscopy is a mature technique with the theory well described and routinely applied in process control, exploration, mining and manufacturing, apart from research and development applications. The "big shrink" as in most analytical technologies was the result of improved electronics and computer chips, and together with the advance of the SDD detector Energy Dispersive XRF was ready to enter the playground. Handheld XRF moved from a metal sorting scanner to an actual quantitative analytical tool. But here lies the biggest challenge, because of reduced cost and ease of operation, this tool is now more accessible to people who often do not have the insight in the limitations.

In this workshop, firstly the differences between analysis in the field vs. the laboratory would be explained, and methods to improve accuracy or interpret the data based on the know inaccuracies. Then some specific Geology case studies will be presented, and lastly we will introduce some case studies in the field of art and conservation where the ability to bring a non-destructive technique to the actual object probably had the biggest impact, but again, not without pitfalls.

The Monday evening XRD poster session will be held 5:00 pm – 7:00 pm in the Westminster foyer, in conjunction with a wine and cheese reception. Three "Best Poster" awards will be given at the end of the session, including "Best Student Poster".
Chair: **T.R. Watkins**, Oak Ridge National Laboratory, USA, watkinstr@ornl.gov

Signifies presenting author, when noted

D-3 **Relative Stability of Anhydrous/hydrated Products of Calcium Chloride during Complete Dehydration as Examined by High-temperature Powder X-ray Diffraction**
K.S.P. Karunadasa*, C.H. Manoratne, Industrial Technology Institute, Sri Lanka
H.M.T.G.A. Pitawala, R.M.G. Rajapakse, University of Peradeniya, Sri Lanka

D-6 **Latest Developments in Non-ambient XRD Attachments from Anton Paar**
A.O.F. Jones*, A. Pein, Anton Paar GmbH, Austria

D-9 **Crystal Structural Analysis of $InAs_xP_{1-x}$ Nanowire Exploiting High Resolution X-ray Diffraction**
S. Song*, C.S. Kim, Korea Research Institute of Standards and Science, Korea

D-11 **Structural Investigation of Plutonium Oxalate Species and Comparison of Their Oxide Products**
J. Corbey*, L. Sweet, D. Meier, A. Casella, PNNL, USA

D-12 **Observation of Crystal Structure Changes with Full Field X-ray Diffraction Imaging Instrument**
M. Yamanashi, Kyoto Municipal Institute of Industrial Technology and Culture, Japan
K. Tsuji, Osaka City University, Japan

D-14 **Fretting Corrosion of Wind Turbine Drivetrains: Causes to Cures using XRD**
J. Brum, Olympus, USA

D-15 **Crystal Structures of Large-Volume Commercial Pharmaceuticals**
J.A. Kaduk*, North Central College, Illinois Institute of Technology and Poly Crystallography, Inc., USA
A.M. Wheatley, North Central College, USA
A.M. Gindhart, T.N. Blanton, ICDD, USA

D-16 **Crystal Structures of Ammonium Citrates**
A.M. Wheatley, J.A. Kaduk*, North Central College, USA

D-23 **Development and Performance Test of X-ray Source for Industrial Benchtop & Handheld XRF**
J.D. Kim*, S.H. Kim, SUNJE R&D Center, Korea
D.H. Lee, Pukyung National University, Korea

D-24 **Prediction of a KIST PIXE/PIGE Facility Based on Design and Simulations**
S.M.T. Hoang, H.N. Tran, Duy Tan University, Vietnam
G.M. Sun, Korea Atomic Energy Research Institute, Korea

D-25 **Validation of the McStas-MCNPX Interface Features in Calculation of Shielding and Gamma/Neutron Backgrounds**
S.M.T. Hoang, H.N. Tran, Duy Tan University, Vietnam
G.M. Sun, Korea Atomic Energy Research Institute, Korea

D-27 **Mineral Analysis of River Sand around Mt. Tsukuba for Provenance Estimation of Atamadai Type Pottery (2500-1500 BC) From Hinoki Site (Tochigi Japan)**
S. Ichikawa*, Y. Sakito, T. Kurisaki, Fukuoka University, Japan

D-29 **Geochemical Analysis of Iron Enriched Soil of Meherrin Virginia**
J. Brum, Olympus, USA
S.I. Chojna, A.M. Sikder, X.C. Liu, L. Kelly, Virginia Commonwealth University, USA

D-30 **BM: a Python Code for Modelling Physically Based Background for XRD**
B. Ramírez, S. García, L. Bucio, Universidad Nacional Autónoma de México, México

The Tuesday evening XRF poster session will be held 5:00 pm – 7:00 pm in the Westminster foyer, in conjunction with a wine and cheese reception. Three "Best Poster" awards will be given at the end of the session, including "Best Student Poster".
Chair: **M. Schmeling**, Loyola University Chicago, USA, mschmel@luc.edu

Signifies presenting author, when noted

F-5   **The Development of Grazing Incidence XAFS and TXRF Method at SSRF XAFS Beamline**
Y. Huang, Shanghai Synchrotron Radiation Facility, Chinese Academy of Sciences, China

F-6   **Potential Environmental Applications by Medium Energy Micro-probe Beamline Proposed in SSRF Phase-II Project**
L. Li, Shanghai Synchrotron Radiation Facility, Chinese Academy of Sciences, China

F-11   **A Novel Approach to the Analysis of Glass Components used in Portable Electronic Devices by Micro-XRF**
J. Vargeson*, K. Eckart, A. Nached, Corning Incorporated, USA

F-16   **Polychromatic Simultaneous WDXRF for Valence Evaluation of Cathode Active Materials in Lithium-ion Batteries**
T. Yoneda*, T. Izumi, S. Tokuda, S. Adachi, K. Sato, Shimadzu Corporation, Japan
M. Kobayashi, T. Mukai, H. Tanaka, M. Yanagida, National Institute of Advanced Industrial Science and Technology, Japan

F-19   **New and Current USGS Shale Reference Materials for Shale Analysis by Energy Dispersive X-ray Fluorescence**
A.R. Orkild-Norton*, S. Wilson, USGS, USA

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A. Ohbuchi*, Applied Rigaku Technologies, USA; Rigaku Corporation, Japan and Meiji University, Japan
W. Matsuda, H. Takahara, S. Ikeda, Rigaku Corporation, Japan
K. Fujii, Y. Koike, Meiji University, Japan

F-23   **Novel X-ray Detector Window for Microanalysis Applications**
J. Abbott, J. Sommer, J. Wong, Moxtek, Inc., USA

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C. Luckey*, G. Becker, R. Bergmann, R. Heil, J. Knobloch, E. Lechner, S. Pahlke, T. Schmid, C. Zacher, KETEK GmbH, Germany

S-13   **X-ray Tomography Using Thin Scintillator Films**
K.E. Kuper, Budker Institute of Nuclear Physics, Russia

F-29   **Silicon Drift Detectors with Improved High Throughput Performance**
M. Zhang*, S. Barkan, J. Wang, V.D. Saveliev, L. Feng, B. Goolsby, E.V. Damron, Hitachi High-Technologies Science America, USA

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S. Cornaby, K. Kozaczek, S. Kamtekar, Moxtek Inc., USA

F-34   **Verification of Wire-Grid Polarizer Coatings Using XRF**
R. Creighton, S. Cornaby, J. Pierce, J. Van Wagoner, S. Kamtekar, J. Rice, B. Naseath, B. Olson, B. Zundel, F. Lane, L. Mounteer, D. Bunting, J. Despain, D. Hammond, Moxtek Inc., USA

F-37   **Optimization of Background Fitting Using Multi-Elemental Reference Materials for XRF Analysis of Air Samples**
S. Yatkin*, K. Trzepla, W. White, N. Hyslop, University of California, Davis, USA
A. Jonkers, Malvern PANalytical, The Netherlands

F-38   **Determination of EDXRF Detection Limits of Air Samples with Custom Low-Loaded Multi-Elemental Reference Materials**
K. Trzepla*, S. Yatkin, W. White, N. Hyslop, University of California, Davis, USA

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F. Mansilla-Koblavi, A.J. N'gouan, J.A. Tenon, Université Félix Houphouët Boigny Cocody Abidjan, Côte d'Ivoire

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Y. Ménesguen, M.C. Lépy, CEA\LNHB, France
W.W. Batista-Pessoa, S. Torrengo, E. Nolot, CEA\LETI, France

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R. Unterumsberger, P. Hönicke, M. Wansleben, M. Müller, B. Beckhoff, Physikalisch-Technische Bundesanstalt, Germany

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N. Gao, XOS, USA
J. Choi, R. Magyar, Bowman XRF, USA

F-49　　**Measure Low Concentrations of Sulfur and Chlorine by MWDXRF**
X. Zhang, F. Wei, Z.W. Chen, X-ray Optical Systems, USA

F-62　　**Characterization of Trace Impurities in 3D Printed Recycled ABS Materials**
Y. Schneider, G. Strossman, EAG Laboratories, USA
O. Keles, A. Cress, San Jose State University, San Jose, USA

F-64　　**Correlation Between XRD Phase Analysis of EAF Slag and Heavy Elements Releasing in Water**
A. Riboldi, L. Borgese*, L.E. Depero, INSTM and University of Brescia, Italy

Minerals and Gems
Chair: T. Blanton, International Centre for Diffraction Data, USA

8:30   **T. Fawcett**, Chairman of the Denver X-ray Conference, Emeritus ICDD, USA

2018 Birks Award - To Be Announced

2018 Jerome B. Cohen Student Award winner to be announced by Chairman of the Cohen Award Selection Committee, **I.C. Noyan**, Columbia University, USA

2018 Robert L. Snyder Student Awards to be announced by **T. Blanton**, Executive Director, ICDD, USA

Remarks by the Plenary Session Chair, **T. Blanton**.

Invited Talks

9:00	P-1	Using X-ray Diffraction to Elucidate Source Materials and Firing Conditions of Pompeian Ceramics **D. Bish***, Indiana University, USA **M. Mercurio, C. Grifa, C. Germinario, A. Langella**, Univ. degli Studi del Sannio, Italy **A. De Bonis, V. Morra, P. Cappelletti**, Univ. degli Studi di Napoli Federico II, Italy
9:45	P-2	Collaborative Mineralogical Research in Museums **A.J. Celestian**, Natural History Museum of LA, USA
10:30		Break
11:00	P-3	New XRD Data Based Approaches to Soil Mineralogy **S. Hillier**, The James Hutton Institute, UK, and Swedish University of Agricultural Sciences, Sweden

Oral Sessions, Wednesday Afternoon, 8 August
Signifies presenting author, when noted

New Developments in XRD & XRF Instrumentation I   Standley I
Chairs: **T. Fawcett**, Emeritus, ICDD, USA, dxcfawcett@outlook.com
A. Drews, Ford Motor Company, USA, adrews@ford.com

1:45	S-10	KETEK's New SDD Generation **M. Fraczek*, F. Dams, R. Fojt, L. Höllt, M. Hofmann, J. Knobloch, N. Miyakawa, A. Pahlke, J. Rumpff, O. Scheid**, KETEK GmbH, Germany
2:00	S-5	Laboratory Source Developments for High Resolution X-ray Microscopy for Higher Throughput, Higher Data Quality and Energy Tunability **M. Feser, R. Ruth, R. Loewen, J. Kasahara, M. Gifford**, Lyncean Technologies, Inc., USA
2:15	S-14	Improved XRF Detector System for High Resolution Spectroscopy in Ambient Air Conditions **H. Schmidt, H. Soltau, A. Niculae, A. Liebel, R. Lackner, D. Steigenhöfer, M. Kopetzky, B. Talbi**, PNDetector GmbH, Germany
2:30	S-26	Claisse® LeDoser-12™ Instrument: How to Save 90% of the Weighing Time in Sample Preparation by Fusion **C. Audet**, Claisse, a Malvern Panalytical brand, Canada
2:45	S-40	True Submicron Resolution X-ray Microscopy of Soft Materials **A. Takase, T.F. McNulty***, Rigaku Americas Corporation, USA

3:00		Break
3:30	S-9	DDM, the new RIR? **T. Degen*, E. Bron, M. Sadki**, Malvern Panalytical, The Netherlands
3:45	S-11	X-ray Nano Computed Tomography Systems and Applications in the Laboratory **D. Murer*, T. Donath**, DECTRIS Ltd., Switzerland **E. Espes, T. Tuohimaa**, Excillum, Sweden **Ch. Fella, S. Zabler**, Fraunhofer IIS, Germany **S. Ferstl**, Technical University Munich, Germany
4:00	S-15	A New Laboratory Diffractometer for Fast PDF Data Collection **T. Hartmann**, Stoe & Cie GmbH, Germany
4:15	S-29	EIGER2 R 500K for the D8 Family **J. Giencke*, B. Jones, N. Henderson, S. Rodesney**, Bruker AXS, USA
4:30	S-41	Product Developments for ICDD® 2019 Powder Diffraction File™ Software **J. Blanton*, R. Vithayathil, C. Karumuhinzi, T. Blanton, S. Kabekkodu, S. Gates-Rector, R. Papoular**, International Centre for Diffraction Data, USA

Microcalorimeter Detectors & Applications   Standley II

Chair: **J. Ullom,** National Institute of Standards & Technology, USA, joel.ullom@nist.gov

1:00		Invited - Resonant X-ray Scattering From Stripe Order in $La_{2-x}Ba_xCuO_4$ Using a TES Detector **P. Abbamonte**, University of Illinois at Urbana-Champaign, USA
1:30	S-7	Invited - Full Chemical Composition Characterization: The Promise of Microcalorimeter Detectors for X-ray Spectroscopy **G.J. Havrilla*, K. McIntosh, M. Croce, M. Rabin**, Los Alamos National Laboratory, USA **F. Vila**, University of Washington, USA **M. Carpenter, R. Cantor**, Star Cryoelectronics, USA
2:00	S-8	A General System for Processing X-ray Microcalorimetry Pulses into Spectra **T. Jach**, National Institute of Standards & Technology, USA **S. Thurgate**, Murdoch University, Perth WA, Australia
2:20	S-32	Table-top Ultrafast X-ray Spectroscopies using a Laser Plasma X-ray Source and Microcalorimeter Sensors **L. Miaja-Avila, G. O'Neil, Y. Il-Joe, D. Swetz, R. Jimenez, J. Ullom**, NIST, USA
2:40	S-33	Realizing the Potential of TES Microcalorimeters for X-ray and Gamma Ray Science at Light Sources **K. Morgan**, National Institute of Standards and Technology, USA
3:00		Break
3:30	S-39	Invited - Ultrasensitive Probing of Local Electronic Structure in the Soft X-ray Regime **D. Nordlund**, SLAC National Accelerator Laboratory, USA
4:00	S-34	Thermal Kinetic Inductance Detectors: Highly Multiplexible Micro-Calorimetric Detectors Not Only for X-ray Imaging Spectroscopy **G. Ulbricht ***, Dublin Institute for Advanced Studies, Ireland **B.A. Mazin, M. Daal**, University of California Santa Barbara, USA
4:20	S-35	A Large-scale Demonstration of TES Microcalorimeters: The SLEDGEHAMMER Gamma-ray Spectrometer **D.T. Becker* , J.A.B. Mates, J. D. Gard, A. Wessels, J.N. Ullom**, University of Colorado, USA **D.A. Bennett, J.W. Fowler, G.C. Hilton, C.D. Reintsema, D.R. Schmidt, P. Szypryt, L.R. Vale, J.N. Ullom**, National Institute of Standards and Technology, USA **M. Croce, A.S. Hoover, K.E. Koehler, M.W. Rabin**, Los Alamos National Laboratory, USA
4:40	S-37	A Cryogen-Free Microcalorimeter Spectrometer for Ultrahigh-Resolution X-ray Microanalysis **R. Cantor**, STAR Cryoelectronics LLC, USA **H. Naito,** HKN Inc., USA

Non-Ambient Cotton Creek

Chair: **S.T. Misture**, NYS College of Ceramics at Alfred University, USA, misture@alfred.edu

1:50	D-54	Invited - Challenges and Rewards Using High-Temperature Diffraction **E.A. Payzant**, Oak Ridge National Laboratory, USA
2:20	S-24	Oxygen Storage Properties and Structural Evolution of AFe_2O_4 (A= Lu, Y, Yb, In) Under Chemical Looping Conditions **R. Jayathilake*, B. Levitas, E. Rodriguez**, University of Maryland, USA
2:40	D-57	Influence of Processing Conditions on Dehydration Kinetics - Use of Non-ambient XRD to Monitor *in situ* Phase Transformations **S. Thakral**, University of Minnesota, USA **J. Garcia-Barriocanal**, University of Minnesota, USA
3:00		Break
3:30	D-5	Invited - *In situ* Neutron Diffraction Studies: Crystal Growth and Ion Exchange **H. zur Loye*, D. Abeysinghe**, University of South Carolina, USA **A. Huq**, Oak Ridge National Laboratory, USA
4:00	D-13	Temperature-dependent X-ray Diffraction of Single-crystal, Epitaxial Films **A.M. Kiefer*, C.J. Reyner, B.B. Claflin**, Air Force Research Laboratory, USA **S.A. Chastang, G.J. Grzybowski**, KBRwyle, USA
4:20	D-17	*In-situ*, Non-ambient Method Development for the Solid State Form Identification of Drug Substance in Drug Product **D. Lievano**, GSK, USA
4:40	D-63	*In-situ* XRD and SEM Study of Ni Colloid Formation from Ni Spinel Oxides **A.C. Ladonis*, B.E. Hill, M. Hall, R. Koch, S.T. Misture**, Alfred University, USA

Industrial Applications of XRF Meadowbrook

Chair: **D. Broton**, Construction Technology Labs, USA, dbroton@ctlgroup.com

1:40	F-25	The Silver Cube Analyser - A High Accuracy On-line Elemental Analyser **J. O'Dwyer*, G. Roach, Y. Van Haarlem, J. Masters**, CSIRO, Australia **J. Tickner**, CSIRO, Crysos Corp., Australia
2:00	F-56	Low Cost Online Real Time Metal Analysis during Pharmaceutical Manufacturing **M. Garcia, N. Kumar**, UHV Technologies, Inc., USA
2:20	F-54	Does Size Matter? Can Portable XRF be used for Process Control? **M. Loubser**, GeoMag GeoChem, South Africa
2:40	F-42	Using XRF to Analyse Impure Gold and Silver (doré) **M. Hinds**, Royal Canadian Mint, Canada
3:00		Break
3:30	F-18	Total Quantification of Mg Alloys by X-ray Fluorescence Spectrometry **W. Matsuda*, A. Morikawa, T. Moriyama**, Rigaku Corporation, Japan **A. Ohbuchi**, Applied Rigaku Technologies, Inc., USA **T. Nakamura**, Meiji University, Japan
3:50	F-22	Optimizing the Mineralogy of a Petroleum Reservoir by Combining Mineral and Elemental Measurements **M. Ammar*, Y. Rocher, E. Colombel, J. Breviere**, Schlumberger Geoservices, France
4:10	F-53	Comparative Study of Chlorine Content Determination in Printed Circuit Boards using a Benchtop XRF and a Handheld XRF **A.R. Wilson, E.C. Gates**, Intel Corporation, USA
4:30	F-35	X-ray Fluorescence and Raman Spectroscopy Data Fusion for Analysis of Duct Tapes: Intra Roll and Inter Product Correlations **S. Mamedov**, HORIBA Scientific, USA

New Developments in XRD/XRF Instrumentation II Standley I

Chairs: **T. Fawcett**, Emeritus, ICDD, USA, dxcfawcett@outlook.com
A. Drews, Ford Motor Company, USA, adrews@ford.com

9:00	S-30	X-ray Diffraction Beamlines in the Brockhouse Sector at the Canadian Light Source

B. Moreno*, N. Appathurai, A. Leontowich, A. Gomez, D. Muir, G. King, B. Yates, Canadian Light Source, Canada
B. Meyer, Brazilian Synchrotron Light Laboratory, Brazil
A. Gomez, S. Kycia, University of Guelph, Canada

9:15	S-27	Development of a Miniature X-ray Emission Spectrometer (miniXES) for Simultaneous Multi-Color Emission Studies of the Non-Resonant X-ray Emission Spectroscopy (XES) , and Sequential Resonant XES for Multiple Edges/Elements

C. Sun*, S. Heald, Argonne National Laboratory, USA
R. Gordon, Simon Fraser Universit, Canada

9:30	S-36	AreX Light: A Benchtop Solution to Retained Austenite Determination

G. Siviero*, L. Seralessandri, G.N.R.S.R.L. Italy

9:45	S-21	The Second Generation of the PROTO AXRD Benchtop Diffraction System

N. Vukotic*, S. Veinberg, PROTO, Canada

10:00		Break

10:30	S-25	Development of a Large-Format Mapping XRF System

A. Drews*, A. Sharafi, W. Paxton, M. Jagner, Ford Motor Company, USA

10:45	S-12	Advanced Pulse Processing Techniques for Energy Dispersive X-ray Photon Science

P. Scoullar, Southern Innovation, Australia

11:00	S-16	Improving Detectors for X-ray Spectroscopy

R. Redus*, A. Huber, R. Dubay, Amptek, Inc., USA

11:15	S-18	Moxtek's Developments in Compact X-ray Sources

S. Cornaby*, T. Parker, R. Steck, B. Harris, K. Kozaczek, C. Smith, E. Miller, S. Kamtekar, Moxtek Inc., USA

Rietveld Standley II

Chair: **J. Kaduk**, Poly Crystallography, Inc. and Illinois Institute of Technology, USA, kaduk@polycrystallography.com

9:00	D-55	Invited - Rebuilding POWGEN: World's Only Third Generation TOF Powder Diffractometer

A. Huq, Oak Ridge National Laboratory, USA

9:30	D-47	Quantification of Correlated Disorder in Alloy Systems Through Complex PDF Modelling

R. Koch, Alfred University, USA

9:50	D-56	Chemical Short-Range Order in Hollandite Type Phases for Nuclear Waste Form Applications

R. Koch, S.T. Misture, Alfred University, USA
J. Amoroso, Savannah River National Laboratory, USA
K. Brinkman, Clemson University, USA

10:10		Break

10:40	D-36	Structural and Texture Refinement of XRD Data of Fluid Catalytic Cracking Catalysts: A Prerequisite Results Requirement to Predict the Steaming Effect on Catalytic Performance

H. Sitepu*, S. Al-Bogami, R.A. Al-Ghamdi, N.M. Al-Yami, Research & Development Center, Saudi Aramco, Saudi Arabia

11:00	D-61	Comparison of Rietveld-Compatible Structureless Fitting Analysis Methods for Accurate Quantification of Carbon Dioxide Fixation in Ultramafic Mine Tailings

C.C. Turvey*, S.A. Wilson, J.L. Hamilton, Monash University, Australia
S.A. Wilson, University of Alberta, Canada
J.L. Hamilton, J. McCutcheon, G. Southam, The University of Queensland, Australia
J. McCutcheon, The University of Leeds, United Kingdom
G.M. Dipple, The University of British Columbia, Canada

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| 11:20 | D-18 | Qualitative and Quantitative Monitoring of Early Age Hydration of Volcanic Ash Blended Cement Using XRF and XRD |
| | | **A. Joseph*, S. Al-Bahar, J. Chakkamalayath**, Kuwait Institute for Scientific Research, Kuwait |

| 11:40 | D-26 | Quantitative Phase Analysis of Samples Containing Low Crystallinity Components by Using the Direct Derivation Method |
| | | **H. Toraya**, Rigaku Corporation, Japan |

Trace Analysis Including TXRF   Cotton Creek

Chair: **L. Borgese**, University of Brescia, Italy, laura.borgese@unibs.it

| 9:00 | F-30 | Invited - Trace Elements Analyses with Synchrotron Radiation Induced X-ray Fluorescence |
| | | **D. Eichert**, Elettra - Sincrotrone Trieste, Italy |

9:30	F-57	Invited - Determination of Gas-Phase Mercury Using TXRF
		U.E.A. Fittschen*, TU Clausthal, Germany
		S. Boettger, TU Clausthal and Europa Univerität Flensburg, Germany

10:00	F-36	TXRF- A Critical Tool to Cleaning Success of NASA Genesis Solar Wind Samples
		M. Schmeling*, Loyola University Chicago, USA
		J.H. Allton, NASA Johnson Space Center, USA
		A.J.G. Jurewicz, Arizona State University, USA
		D.S. Burnett, California Institute of Technology, USA

| 10:20 | | Break |

| 10:50 | F-12 | New Sample Preparation for TXRF Analysis Using Resist Pattern Layer |
| | | **K. Tsuji*, T. Furusato, N. Yomogita**, Osaka City University, Japan |

11:10	F-28	X-ray Fluorescence Spectrometry Beamline at Elettra Sincrotrone Trieste: Perspectives for Trace Element Analysis in Material Science and Environmental Applications
		M. Czyzycki*, I. Bozicevic-Mihalic, G. Aquilanti, Elettra-Sincrotrone Trieste, Italy
		A.G. Karydas, J.J. Leani, A. Migliori, J. Osan, M. Bogovac, P.M. Wrobel, M. Sibilia, I. Darby, R.B. Kaiser, International Atomic Energy Agency, Austria
		M. Kokkoris, National Technical University of Athens, Greece

Cultural Heritage   Standley I

Chairs: **R. Van Grieken**, University of Antwerp, Belgium, rene.vangrieken@uantwerpen.be
M. Schmeling, Loyola University Chicago, USA, mschmel@luc.edu

2:00	F-51	Invited - Scanning X-ray Powder Diffraction Mapping of Painted Works of Art using Cu and Ag Lab Sources: Advantages and Limitations **F. Vanmeert, S. De Meyer, G. Van der Snickt, K. Janssens***, University of Antwerp, Belgium
2:30	F-58	Invited - Travelling through Space and Time: A Novel MA-XRF Imaging Method for Separating Sources of Chemical Information in Large Works of Art **G. Pastorelli*, E. Pouyet, M. Walton**, Northwestern University/Art Institute of Chicago, USA **N. Rohani, O. Cossairt, A. Katsaggelos**, Northwestern University, USA **K. Smith, K. Eremin**, Harvard Art Museums/Straus Center for Conservation, USA
3:00		Break
3:30	F-21	A New Tool for Cultural Heritage: High Speed, Simultaneous XRD-XRF Mapping with the Color X-ray Camera **J. Davis, J. Schmidt, M. Huth, H. Soltau**, PNDetector, GmbH, Germany **R. Hartmann, L. Strüder**, PNSensor, GmbH, Germany
3:50	D-22	Difractometric Analysis as a Toll for an Early-Byzantine Stone Tesserae Origin, on the Example of a Mosaic from the Basilica in Chhim (Lebanon) **A. Tomkowska***, Academy of Fine Arts in Warsaw, Poland **M. Ruszkowski**, University of Warsaw, Poland

General XRD   Standley II

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

2:00	D-20	Invited - Implementation of the Self-consistent Kröner-Eshel by Model for the Calculation of X-ray Elastic Constants for any Crystal Symmetry **A. Vermeulen*, N. Norberg**, Malvern Panalytical, Netherlands **C. Kube**, Bennett Aerospace, USA
2:30	D-4	The Kepler Tiling as the Oldest Complex Surface Structure in History: X-ray Analysis of a Two-Dimensional Oxide Quasicrystal Approximant **H.L. Meyerheim*, S. Roy, K. Mohseni**, Max-Planck-Institut fuer Mikrostrukturphysik, Germany **S. Förster, F. Schumann, M. Trautmann, E.M. Zollner, W. Widdra**, Martin-Luther-Universität Halle-Wittenberg, Germany
2:50	D-37	Crystal Structure, Texture and Phase Composition of Metal Orthovanadates and Nickel Vanadates Investigated by XRD and the Rietveld Method **H. Sitepu*, A. Akah, T. Inan, R.A. Al-Ghamdi**, Saudi Aramco, Saudi Arabia
3:10		Break
3:30	D-62	Machine Learning Tools for Diffraction Data Analysis **M. Ragni, P. Bosetti, M. Leoni***, University of Trento, Italy
3:50	D-19	Synthesis and Characterisation of High Entropy Alloys **J. Menghani*, S. Patel**, S.V. National Institute of Technology, India
4:10	D-7	Healing X-ray Scattering Images **J. Liu*, J. Lhermitte, Y. Tian, Z. Zhang, K. Yager**, Brookhaven National Laboratory, USA **D. Yu**, Brookhaven National Laboratory and New Jersey Institute of Technology, USA
4:30	D-41	Alternative Concepts for Beam Monochromatization **D. Beckers*, M. Gateshki, D. J. Götz**, Malvern Panalytical, The Netherlands

Advanced Fundamental Parameters   Cotton Creek

Chair: **J. Ullom**, National Institute of Standards & Technology, USA, joel.ullom@nist.gov

2:00	F-32	Invited - Advances in SI-Traceable Wavelength Metrology

C.I. Szabo*, Theiss Research and NIST, USA
L.T. Hudson, M.H. Mendenhall, A. Henins, J.P. Cline, NIST, USA

2:30   F-50   Invited - The Use of Fundamental Parameters in XRF – An Industry Perspective
B. Vrebos*, P. Brouwer, Malvern Panalytical, The Netherlands

3:00   Break

3:30   F-39   New Measurements of X-ray Mass Attenuation Coefficients
Y. Ménesguen*, M.-C. Lépy, CEA, France
B. Beckhoff, PTB, Germany

3:50   F-45   Atomic Fundamental Parameter Determinations at PTB using Well-Known Synchrotron Radiation and Calibrated Instrumentation
B. Beckhoff*, P. Hönicke, I. Holfelder, Y. Kayser, M. Kolbe, J. Lubeck, M. Müller, B. Pollakowski-Herrmann, R. Unterumsberger, J. Weser, Physikalisch-Technische Bundesanstalt (PTB), Germany

4:10   F-52   Superconducting Microcalorimeters for X-ray Spectroscopy
J. Fowler, NIST Boulder Labs, USA

4:30   F-65   High-Precision Reference-Free Measurements of Soft X-ray Transitions with a Double Crystal Spectrometer
J. Machado*, Universidade Nova de Lisboa, Portugal and Sorbonne Université, France
J.P. Santos, P. Amaro, M. Guerra, Universidade Nova de Lisboa, Portugal
J.M. Isac, P. Indelicato, Sorbonne Université, France
C.I. Szabo, Theiss Research and NIST, USA
A. Gumberidze, GSI Helmholtzzentrum für Schwerionenforschung, Germany
G. Bian, Sorbonne Université, France and Sichuan University, China

General XRF   Meadowbrook

Chairs: **U.E.A. Fittschen**, TU-Clausthal, Germany, ursula.fittschen@tu-clausthal.de
         S. Vaidya, CTLGroup, USA, svaidya@ctlgroup.com

2:00   F-9   Invited - XRF: Capabilities for Analytical Problem Solving
G. Havrilla, Los Alamos National Laboratory, USA

2:30   F-13   Invited - Applications of XRF and XRD for the Characterization of Coal Fly Ash for Use in Construction Products
A. Joshi*, E.I. Diaz-Loya, C. Sieg, R. Minkara, Boral Resources, USA

3:00   Break

3:30   F-55   Fast X-ray Sorting for Recycling Light Metals
M. Garcia*, N. Kumar, UHV Technologies, Inc., USA

3:50   F-17   Inclusion of the Radiative Auger Effect X-ray Emission Spectra in Fitting K-spectra of Elements in the Range Z = 26-35
B. Ganly*, S. Peacock, Y. Van Haarlem, CSIRO, Australia
S. Hughes, University of Wollongong, Australia

4:10   F-14   Solid Analysis Techniques to Monitor Metals in Plastic Packaging for Pharmaceuticals
S. Wood*, L. Breckenridge, N. Lewen, Bristol-Myers Squibb, USA

4:30   F-59   Using Wavelength-Dispersive X-ray Fluorescence (WD-XRF) as a Walkup, High-throughput Alternative to Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES) for R&D Pharmaceutical Elemental Impurity Applications
T.M. Brucker*, E.J. Borsje, H.T. Rasmussen, Vertex Pharmaceuticals, Inc., USA

Oral Sessions, Friday morning, 10 August

Imaging   Meadowbrook

Chairs: **K. Tsuji**, Osaka City University, Japan, tsuji@a-chem.eng.osaka-cu.ac.jp
F. Meirer, Utrecht University, The Netherlands, f.meirer@uu.nl

8:30	S-6	Invited - Novel Reflective Optics and Systems for Hard X-ray Microscopy **K. Yamauchi**, Osaka University, Japan

9:00	S-17	Liquid-Metal-Jet and High-Resolution X-ray Source Technology for Imaging **J. Hallstedt, O. Hemberg, G. Johansson, B. Hansson**, Excillum AB, SWEDEN **A. Adibhatla**, Excillum Inc, USA

9:20 S-19 120 kV & 5 Watt Compact X-ray Source
E. Miller, S. Cornaby, G. Smith, R. Steck, B. Harris, K. Kozaczek, S. Kamtekar, Moxtek Inc., USA

9:40 Break

10:00 S-38 Invited - X-ray Microfluorescence Imaging of Samples from Deep Earth to Interstellar Space
L. Vincze, Ghent University, Belgium

10:30 S-20 Invited - Spectro-microscopy and Nano-tomography with Transmission X-ray Microscopy
J. Nelson Weker, SLAC National Accelerator Laboratory, USA

11:00 S-22 3D Imaging of Geological Materials using X-ray Diffraction and Spectroscopy
M.K.A. Koker*, M. Newville, A. Lanzirotti, GSECARS, University of Chicago, USA

Advanced Methods   Standley I

Chairs: **T.R. Watkins**, Oak Ridge National Laboratory, USA, watkinstr@ornl.gov
M.A. Rodriguez, Sandia National Laboratory, USA, marodri@sandia.gov

8:30 D-73 Invited - Residual Stress Measurements in Additively Manufactured Stainless Steel Valve Housing
B. Clausen*, D.W. Brown, Los Alamos National Laboratory, USA
J.E. Bishop, K. Johnson, B. Jared, K. Allen, D. Balch, A. Roach, Sandia National Laboratory, USA

9:00 D-39 Invited - Bulk Texture Measurements with the Neutron Time-of-Flight Diffractometer HIPPO
S.C. Vogel, LANL, USA

9:30 D-33 Depth-Resolved Monochromatic Nanobeam X-ray Diffraction for Evaluation of Local Strain in Single
Crystalline Samples using Differential Aperture Method
Y. Imai*, K. Sumitani, S. Kimura, Japan Synchrotron Radiation Research Institute (JASRI), Japan
K. Shida, S. Takeuchi, A. Sakai, Osaka University, Japan

9:50 D-21 The Gandolfi Stage: A Novel Approach for the Analysis of Single Crystals and Small Volume Samples
G. Schmidt, Thermo Scientific, USA

10:10 Break

10:30 S-28 Invited - Use of XRD and PDF Analysis to Define the Roles of Defects in Electrochemical Charge Storage
S. Misture*, R. Koch, P. Metz, M. Flint, P. Gao, Alfred University, USA

11:00 S-31 In Operando Characterization of Li-Ion Battery Materials
S.N. Rodesney*, N. Yang, N. Henderson, J. Giencke, B. Jones, Bruker AXS, Inc., USA

11:20 D-35 Microstructural Properties of Plutonium Oxalates and Oxides as a Function of Processing Conditions
L. Sweet*, J. Corbey, A. Casella, M. McCoy, K. Pitts, Pacific Northwest National Laboratory, USA
M. Leoni, University of Trento, Italy

11:40 D-75 Atomic-level Perspective on the Functionality of Nanoalloy Catalysts Inside Operating Fuel Cells by
Combined in Operando High Energy X-ray Spectroscopy and Total Scattering
Y. Maswadeh, Central Michigan University, USA

Industrial Applications of XRD   Standley II

Chair: **I.C. Noyan**, Columbia University, USA, icn2@columbia.edu

8:30	D-53	Invited - Quantitative XRD & XRF Analyses: Unified and Simplified **F.H. Chung**, Sherwin-Williams Research Center, USA
9:00	D-38	Quantitative Phase Analysis of XRD Data of Sludge Deposits from Refineries and Gas Plants by Use of the Rietveld Method **R.A. Al-Ghamdi*, H. Sitepu**, Saudi Aramco, Saudi Arabia
9:20	D-28	XRD Analysis of Illite-Smectite Interstratification in Clays from Oil Sands Ores **B. Patarachao**, National Research Council, Canada
9:40	D-46	Quantification of Cement Phases and Cement Replacement Materials by Rietveld Refinement Starting from Hydrated Cement Phases in Non-Ambient Conditions **S.T. Witzleben*, K. Walbrück**, Bonn-Rhein-Sieg University, Germany **F. Mundo**, University of Palermo, Italy
10:00		Break
10:20	D-65	Invited - Applications of XRD at Ford Motor Company **W.A. Paxton*, M. Jagner, A. Drews**, Ford Motor Company, USA
10:50	D-48	Quantitative Analysis of Pt on Industrially-Relevant Catalyst Supports **E.J. Peterson*, A. DeLaRiva, D. Kunwar, G. Canning, C.R. Riley, A.K. Datye**, The University of New Mexico, USA
11:10	D-64	Characterization and Phase Identification of Metals, Alloys, and Corrosion Materials using the Powder Diffraction File™ **T. Blanton**, ICDD, USA
11:30	D-68	Characterization of Pharmaceutical Formulations by X-ray Powder Diffraction **T. Fawcett***, Emeritus ICDD, USA **S. Gates-Rector, A. Gindhart, T. Blanton, J. Blanton**, ICDD, USA

Quantitative Analysis of XRF   Cotton Creek

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

8:30	F-63	Invited - A Versatile Fundamental Parameter Software for Quantification in XRF Considering Various Spectral Modification Modes Including X-ray Optics **P. Wobrauschek*, P. Necker, B. Großmayer, C. Streli**, Atominstitut, TU Wien, Austria
9:00	F-60	Invited - Evaluating Perspectives from the Past Missions to Shape Future Investigations using the Mars 2020 Planetary Instrument for X-ray Lithochemistry **C.M. Heirwegh*, A.C. Allwood, D.T. Flannery, Y. Liu**, Jet Propulsion Laboratory, California Institute of Technology, USA **J.A. Hurowitz**, Stony Brook University, USA **B.C. Clark**, Space Science Institute, USA
9:30	F-44	Hindsight 2020: The Challenges of X-ray Spectroscopy on Mars **R. Gellert**, University of Guelph, Canada
9:50	F-10	Preparation of Liquid Samples using Nanoimprint Film and Quantitative Analysis of Mineral Component by Fundamental Parameter Method **Y. Konyuba*, H. Onodera**, JEOL Ltd., Japan **T. Yahagi**, Yamagata Research Institute of Technology, Japan
10:10		Break
10:30	F-27	Invited - Full Spectrum Modeling: Understanding the Matter **T. Wolff*, F. Reinhardt**, Bruker Nano, Germany **F. Nitsche**, Bruker AXS, Germany **D. Docenko**, Free consultant, Israel
11:00	F-24	Coherent Normalization for *in vivo* Bone Lanthanum XRF Measurements **J. Nguyen, A. Pejovic-Milic, J. Grafe***, Ryerson University, Canada
11:20	F-31	Cross and Internal Comparisons: Integrative and Parametric Approaches to X-ray Fluorescence Data Analysis and Processing **A.M. Crawford*, G.N. George, I.J. Pickering**, University of Saskatchewan, Canada **A. Deb, J.E. Penner-Hahn**, University of Michigan, USA

11:40   F-46   SI Traceable Characterization of Nanomaterials by X-ray Spectrometry
B. Beckhoff*, P. Hönicke, I. Holfelder, Y. Kayser, B. Pollakowski-Herrmann, C. Seim, C. Streeck, R. Unterumsberger, M. Wansleben, J. Weser, C. Zech, Physikalisch-Technische Bundesanstalt (PTB), Germany

	Standley I	Standley II	Cotton Creek	Meadowbrook (Lake House when noted)

Monday Morning Workshops 9:00 am – 12:00 Noon

	Meeting Rooms			
	Standley I	**Standley II**	**Cotton Creek**	**Meadowbrook (Lake House when noted)**
XRD	Material Identification – The good, bad & ugly (**Fawcett**)			Selecting Software for Rietveld Refinement I (**Yakovenko**) Lake House
XRF		Basic XRF (**Anzelmo**)	Quantitative Analysis of XRF I (**Elam**)	

Monday Afternoon Workshops 1:30 pm – 4:30 pm

XRD	Quantitative Phase Analysis (**Ryba**)	Two-Dimensional Detectors (**He/Blanton**)		Selecting Software for Rietveld Refinement II (**Yakovenko**) Lake House
XRF			Quantitative Analysis of XRF II (**Elam**)	Energy Dispersive XRF (**Lemberge**)

Monday Evening XRD Poster Session & Reception 5:00 pm – 7:00 pm. (Watkins) [Westminster Foyer]

Tuesday Morning Workshops 9:00 am – 12:00 Noon

Special Topic	Characterization of Thin Films (**Hradil**)			
XRD		Line Profile Analysis (**Leoni**)		
XRF			Micro XRF (**Zaitz**)	Sample Preparation of XRF (**Anzelmo**)

Tuesday Afternoon Workshops 1:30 pm – 4:30 pm

Special Topic	Imaging (**Vogt**)			
XRD		Non-Ambient (**Misture**)		
XRF			Trace Analysis (**Streli/Wobrauschek**)	Handheld XRF – The Silver Bullet or Fools Gold? (**Loubser**)

Tuesday Evening XRF Poster Session & Reception 5:00 pm – 7:00 pm. (Schmeling) [Westminster Foyer]

Wednesday Morning Plenary Session, Minerals and Gems
Standley I&II, 8:30 am – 11:45 am (Blanton)

Wednesday Afternoon Sessions

Special Topic	New Developments in XRD & XRF Instrumentation I (**Fawcett**)	Microcalorimeter Detectors & Applications (**Ullom**)		
XRD			Non-Ambient (**Misture**)	
XRF				Industrial Applications of XRF (**Broton**)

Wednesday Evening Vendor Sponsored Reception 5:30 pm - 7:00 pm. Exhibit Hall

Thursday Morning Sessions

Special Topic	New Developments in XRD & XRF Instrumentation II (**Fawcett**)			
XRD		Rietveld (**Kaduk**)		
XRF			Trace Analysis including TXRF (**Borgese**)	

Thursday Afternoon Sessions

Special Topic	Cultural Heritage (**Van Grieken/Schmeling**)			
XRD		General XRD (**Murray**)		
XRF			Advanced Fundamental Parameters (**Ullom**)	General XRF (**Fittschen/Vaidya**)

Friday Morning Sessions

Special Topic				Imaging (**Tsuji/Meirer**)
XRD	Advanced Methods (**Watkins/Rodriguez**)	Industrial Applications of XRD (**Noyan**)		
XRF			Quantitative Analysis of XRF (**Brehm**)	

Tuition Waiver Opportunities for ICDD XRF & XRD Educational Events

2017/2018
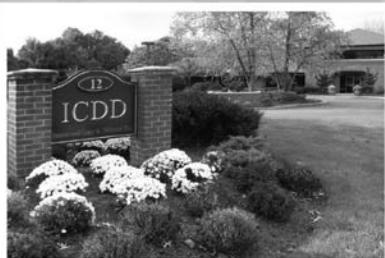
Educational Events

In continuing its commitment to education throughout the scientific community, the International Centre for Diffraction Data sponsors clinics and workshops in X-ray powder diffractometry and X-ray fluorescence spectrommetry. These courses offer training in both theoretical and practical applications.

To promote these clinics and workshops, particularly in the academic sector, the ICDD offers a limited number of tuition waivers. The XRF, XRD I & II, and Rietveld Refinement tuition waivers are named in honor of world-renown scientists Dr. Eugene P. Bertin, Dr. Ron Jenkins, Dr. Deane K. Smith and William Frank McClune.

Who Should Apply

Faculty members and graduate students are encouraged to apply. If you are currently developing a program in X-ray fluorescence (XRF), X-ray powder diffraction (XRD), or Rietveld Analysis, or are interested in incorporating the topic into an established course, a tuition waiver can provide you the opportunity to learn the principles and practices of this discipline from some of the experts in the field.

Restrictions

Tuition waivers cover tuition only; travel and lodging are the responsibility of the attendee and are not included in the tuition waiver.

How to Apply

Submit a one-page written request stating your objectives in attending the clinic or workshop, and/or how you will incorporate the respective topic into the curriculum at your learning institute.

Tuition waiver applications must be accompanied by a clinic/workshop registration form and received at the ICDD by the application and registration deadline. All applications will be reviewed on a competitive basis, and recipients will be notified no later than four weeks prior to the start of the clinic/workshop session.

2017/2018 Applicable Events

Rietveld Refinement & Indexing 1 & 2
25-29 September 2017
Application Deadline: 14 August 2017

Practical XRF
30 April - 4 May 2018
Application Deadline: 18 March 2018

Fundamentals of XRD
4-8 June 2018
Application Deadline: 22 April 2018

Advanced Methods in XRD
11-15 June 2018
Application Deadline: 22 April 2018

Please return a completed registration form and your tuition waiver request to:

ICDD Clinics
12 Campus Boulevard,
Newtown Square, PA 19073

Attention: Eileen Jennings
Email: clinics@icdd.com
www.icdd.com/education

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