

PROGRAM

62nd Annual Conference on Applications of X-ray Analysis
The Denver X-ray Conference

5-9 August 2013

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



Plenary Session

The 100th Anniversary of X-ray Spectroscopy





Training & Applications
Techniques & Instrumentation
Exhibits, Workshops, Sessions
Free CD of the Proceedings

Sponsored by International Centre for Diffraction Data







Up-to-date information can be found on the Denver X-ray Conference web page at http://www.dxcicdd.com. Please continue to monitor this site for the latest conference information. For additional information, contact: Denise Flaherty: Phone: 610.325.9814, Fax: 610.325.9823

Email: flaherty@icdd.com

2013 DENVER X-RAY CONFERENCE PROGRAM-AT-A-GLANCE & MONDAY-FRIDAY & 5-9 AUGUST

Monday N	Norning Workshops 9:00 am – 12:0			
		Meeting		
	Standley Ballroom I	Standley Ballroom II	Cotton Creek	Meadowbrook
XRD		Introduction to the new GSAS-II Crystallographic Analysis System I (Toby/Von Dreele)		Basic to Intermediate XRD Analysis (Misture/Blanton)
XRF	Basic XRF (Elam)		Trace Analysis (Wobrauschek/Streli)	
	Afternoon Workshops 1:30 pm – 4:3	0 pm		
XRD & XRF			X-ray Optics (Fittschen/Havrilla)	
XRD		Introduction to the new GSAS-II Crystallographic Analysis System II (Toby/Von Dreele)		Total Pattern Analysis (Fawcett/Kaduk)
XRF	Energy Dispersive XRF (Phillips)			
Monday E	Evening XRD Poster Session & Rec	eption 5:30 - 7:30 pm; Sponsored by	y ICDD. Westminster Foyer (Watk	ins)
Tuesday N	Morning Workshops 9:00 am – 12:0	0 Noon		
XRD & XRF	Fundamentals of Digital Signal Processing and X-ray Detectors (Hayakawa)			
XRD			Hands-on Rietveld Analysis (Payzant)	Modeling & Analysis of Small- angle Scattering I (Landes/Havsky)
XRF		Quantitative Analysis I (Mantler)		17-
Tuesday A	Afternoon Workshops 1:30 pm – 4:3	30 pm		
XRD		i	Introduction to Volume H (Kaduk)	Modeling & Analysis of Small- angle Scattering II (Landes/Ilavsky)
XRF	Sample Preparation of XRF (Anzelmo)	Quantitative Analysis II (Mantler)		160
Tuesday E	Evening XRF Poster Session & Rec	eption 5:30 - 7:30 pm; Sponsored by	y Chemplex. Westminster Foyer (Va	an Grieken/Zaitz)
		n – 12:00 pm. The 100 th Anniversary	y of X-ray Spectroscopy (Havrilla)	Standley Ballroom
	y Afternoon Sessions			
XRD & XRF	New Developments in XRD & XRF Instrumentation (Fawcett/Blanton) 1:15-5:00			
XRD			High Energy XRD (Almer) 1:30-4:40	
XRF		Quantitative Analysis (Brehm) 1:30-5:00	1.30-4.40	
Wednesda	y Evening Vendor Sponsored Rece	ption 5:30 pm - 7:00 pm; Exhibit Ha	all/Westminster Ballroom	
	Morning Sessions			
XRD & XRF		Applications of XRD & XRF in the Petroleum Industry (Simon/Morton/Doyle) 9:00-11:50		
XRD			Stress Analysis (Brown/Watkins) 8:00-11:50	Pair Distribution Function (Ehm 9:00-11:30
XRF	Applications for Portable XRF (Russell/Benzel) 9:10-11:30			
	Afternoon Sessions	1	L. P. IV.	
XRD & XRF			Applied Materials Analysis (Fawcett/Blanton) 1:00-5:10	
XRD			, , , , , , , , , , , , , , , , , , , ,	Polymers (Liu) (1:30-4:45)
XRF	Fusion & Industrial Applications of XRF (Anzelmo/Thomas) 1:30-4:30	Micro XRF (Havrilla) 1:50-5:10		
Friday Mo	orning Sessions	<u></u>		
XRD		New Developments in Rietveld Analysis (Suchomel) 8:30-11:10		
XRF	Trace Analysis (Zaitz) 8:30-11:50			

 $ICDD, the \ ICDD \ logo \ and \ the \ Denver \ X-ray \ Conference \ and \ Design \ are \ registered \ in \ the \ U.S. \ Patent \ and \ Trademark \ Office.$

AM Workshops 9:00 AM-12:00 PM | PM Workshops 1:30 PM-4:30 PM

MONDAY AM

XRD

INTRODUCTION TO THE NEW GSAS-II CRYSTALLOGRAPHIC ANALYSIS SYSTEM—FULL DAY | Standley Ballroom II Organizers & Instructors:

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

The workshop will introduce the attendees to the use of the new GSAS-II software package for the reduction, solution and refinement with all types of X-ray and neutron crystallographic data. The workshop will emphasize work with powder diffraction data. All software needed to install and run the software is freely available. Attendees will be expected to bring their own laptops with the software already downloaded. The workshop will be targeted towards individuals with some experience with Rietveld analysis and to experienced single-crystal crystallographers with some knowledge of powder diffraction. Areas to be covered include use of GSAS-II for: area detector data integration, indexing patterns, structure solution by charge-flipping, and Rietveld refinement with constraints and restraints.

BASIC TO INTERMEDIATE XRD ANALYSIS | Meadowbrook

Organizers & Instructors:

Thomas N. Blanton, Eastman Kodak Company, Rochester, NY, USA, thomas.blanton@kodak.com

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

Thomas R. Watkins, Oak Ridge National Laboratory, Oak Ridge, TN, USA

Mark A. Rodriguez, Sandia National Laboratory, Albuquerque, NM, USA

The use of XRD in routine qualitative and non-Rietveld quantitative analysis will be presented. The use of XRD in phase identification will be covered, including introductory remarks on sample preparation and a discussion of common XRD geometries. Next, we will cover profile fitting and lattice parameter refinement for determination of the composition of solid solutions via Vegard's law. Finally, we will cover the use of the reference intensity ratio method for semi-quantitative analysis and full quantification using the internal standard method.

XRF

BASIC XRF || Standley Ballroom I

Organizer & Instructors:

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

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

A.R. Drews, Ford Motor Company, Dearborn, MI, USA

This workshop provides a basic introduction to the principles of XRF, and is specifically aimed at those new to the field. It will start with a general overview of the technique, followed by more specific details of the basic principles. The emphasis will be on understanding how to use XRF and what its capabilities are. In the second half of the workshop, a few selected applications will be presented. The focus of this segment will be to provide an understanding of how the basic principles affect actual practice.

TRACE ANALYSIS | Cotton Creek

Organizers & Instructors:

C. Streli, TU Wien, Atominstitut, Wien, Austria, streli@ati.ac.at

P. Wobrauschek, TU Wien, Atominstitut, Wien, Austria, wobi@ati.ac.at

K.Tsuji, Osaka City University, Osaka, Japan

A. Martin, Thermo Fisher Scientific, Sugarland, TX, USA

Both beginners and experienced X-ray physicists will gain information by attending the Trace Analysis workshop. Presentations of most modern techniques and instrumentation for trace element analysis using WDXRF, EDXRS, and more will be given. Physical methods to improve minimum detection limits in XRF by background reduction will be discussed; examples of synchrotron radiation as an excitation source, as well as standard WDXRF laboratory instrumentation. 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 (e.g., Carbon). Confocal µ-XRF will be presented as a 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 and the importance of the various XRF spectrometric techniques. Trace analysis techniques by WDXRF – methods and pitfalls: background selection, crystal and collimator options, sample types and more will be discussed.

MONDAY PM

XRD & XRF

X-RAY OPTICS || Cotton Creek

Organizers & Instructors:

U. Fittschen, Universität Hamburg, Hamburg, Germany, ursula.fittschen@chemie.uni-hamburg.de

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

G. Wellenreuther, HASYLAB at DESY, Hamburg, Germany

M. Kraemer, AXO Dresden GmbH, Dresden, Germany

This workshop will focus on the different state-of-the-art focusing X-ray optics. Capillary optics, DCC-Optics, Fresnel Zone Plates, KB-mirrors and compound refractive lenses will be covered. Their capability and performance will be illustrated with examples from latest research results from laboratory-based instrumentation and synchrotron facilities. The workshop level will be appropriate for beginners and advanced beginners addressing also the underlying physical principles like refraction, diffraction and total reflection.

XRD

INTRODUCTION TO THE NEW GSAS-II CRYSTALLOGRAPHIC ANALYSIS SYSTEM—CONTINUED

Organizers & Instructors:

Standley Ballroom II

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

TOTAL PATTERN ANALYSIS | Meadowbrook

Organizers & Instructors:

T. Fawcett, International Centre for Diffraction Data, Newtown Square, PA, USA, fawcett@icdd.com

J.A. Kaduk, Poly Crystallography, Inc., Naperville, IL, USA, kaduk@polycrystallography.com

Total pattern analysis (TPA) is fundamentally a concept whereby all possible available information can be derived from a powder diffraction pattern. This would include the identification of all materials present in the specimen, information about the crystalline state of each material, the crystallite size, stress, strain, particle size, shape, etc. Several different approaches have been used to perform TPA analyses. One approach is to mathematically deconvolute the pattern and analyze each contributing component by using fundamental parameters and diffraction physics. This approach has been commonly used for highly crystalline materials. TPA can also be performed empirically by using simulations of digitized experimental components and this approach is frequently used for non-crystalline materials, mixtures having a noncrystalline component, or in cases where the fundamental parameters are not known. Several recent methods give the user a choice of several approaches that can be mixed depending upon the nature of the specimen being analyzed and information being sought. In this workshop we will review various methods for performing TPA analyses and discuss the fundamental strengths and weaknesses of various approaches.

XRF

ENERGY DISPERSIVE XRF || Standley Ballroom I

Organizer & Instructors:

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

R. Cone, Consultant, Orlando, FL, USA

A. McWilliams, RTI International, Research Triangle Park, NC, USA

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.

TUESDAY AM

XRD & XRF

FUNDAMENTALS OF DIGITAL SIGNAL PROCESSING AND X-RAY DETECTORS | Standley Ballroom I

Organizer & Instructors:

S. Hayakawa, Hiroshima University, Hiroshima, Japan, hayakawa@hiroshima-u.ac.jp

J. Kawai, K. Ohira, Kyoto University, Kyoto, Japan

S. Terada, X-Bridge Technologies, Kyoto, Japan

T. Papp, Cambridge Scientific, Ontario, Canada

This workshop will introduce various X-ray detectors (Si, Ge, and CdTe SSD, SDD, Si-PIN, proportional counter) and explain what is done in the digital signal processors of X-ray spectrometers is explained. The workshop covers (1) basics of DSP (digital signal processor) and digital oscilloscope, (2) deadtime correction, (3) peak stability and calibration, (4) linear and nonlinear response, (5) low-energy tail, (6) trade-offs among energy resolution, throughput and effective area, (7) escape peaks, sum peaks, and pile-up signals, (8) Fano factor, (9) how to determine the best set of parameters, and (10) near room temperature operation.

XRD

HANDS-ON RIETVELD ANALYSIS | Cotton Creek

Organizer & Instructors:

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

P. Zavalij, University of Maryland, College Park, MD, USA

Objective: Attendees will have the opportunity to refine experimental X-ray and neutron data sets. The instructors will present a series of worked examples to illustrate important issues in Rietveld refinement.

Topics to be addressed will include:

- Recommended refinement strategies
- · Refinement indices and what they mean
- Structure models and instrumental parameters
- · How to use the program to model a hypothetical pattern
- How to refine: lattice parameters, site occupancy factors,
 Quantitative analysis and amorphous content thermal parameters, preferred orientation
- How to properly consider instrumental parameters
- · What to do for an incomplete structure model

Accuracy and precision

Attendees are encouraged to bring laptop computers with Rietveld software installed. Data files will be provided. In the workshop, these data files will be refined using the free program GSAS with the EXPGUI, but other popular programs (FullProf, Topas, Jade, High-Score, MAUD, Rietan, etc.) will be discussed during the workshop.

Software: GSAS with EXPGUI is available from: https://subversion.xor.aps.anl.gov/trac/EXPGUI

Reference (optional): Fundamentals of Powder Diffraction and Structural Characterization of Materials, VK Pecharsky and PY Zavalij, Springer

MODELING & ANALYSIS OF SMALL-ANGLE SCATTERING—FULL DAY // Meadowbrook

Organizer & Instructor:

B. Landes, Dow Chemical Company, Midland, MI, USA, bglandes@dow.com

J. Ilavsky, Argonne National Laboratory, Argonne, IL, USA, ilavsky@aps.anl.gov

Successful small-angle X-ray and neutron scattering (SAXS & SANS) experiments require appropriate data analysis tools. Various tools were developed over the years, for example ATSAS, mostly applicable for biological systems and NIST Analysis package for Igor Pro. For complex problems in materials science, physics, and chemistry, Igor Pro based package Irena was developed during the last 12 years at the APS. It is being widely used for support of SAXS and USAXS beamlines at the APS and number of other facilities worldwide. Six courses on how to use this package were made available to the SAXS/SANS community just during the last 12 months in the US, Australia, and Brazil. The course will be taught by the software author, Jan Ilavsky, APS staff member. The course will walk users through the use of the selected tools in this package from data import, manipulation & graphing, to different methods of analysis and export of the results. Theories behind the tools and their correct applicability to various problems will be discussed. Participants are expected to bring their computers (Windows or Mac OS). A demo version of Igor 6 will be provided to users (if needed) as well as CD with copy of the latest SAXS software version and other materials. In addition, participants are encouraged to bring their own SAXS experimental results for discussions if time is available.

About the software: Irena is a package of tools for analysis of small-angle scattering (SAXS, SANS, USAXS, USANS) data. For more details on this software package please visit: http://usaxs.xray.aps.anl.gov/staff/ilavsky/irena.html

XRF

QUANTITATIVE ANALYSIS—FULL DAY | Standley Ballroom II

Organizer & Instructors:

M. Mantler, Rigaku Corporation, Japan, michael.mantler@rigaku.com

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

B. Vrebos, PANalytical B.V, Almelo, The Netherlands

Morning: Basic methods and resources

- 1. Classical fundamental parameters and mathematical models.
- 2. Empirical and theoretical influence coefficients.
- 3. Fundamental parameter collections and tube spectra: Sources, availability, and reliability.
- 4.A free Excel-tool for comparison of fundamental parameter data and simple computations.

Afternoon: Advanced methods.

- I. Compensation methods (standard addition, internal standard, heavy absorber, Compton scattering).
- 2. Layered materials, inhomogeneous samples, and rough surfaces.
- 3. Light elements. Heavy elements in a light matrix. Trace element analysis. Analysis using L- and M-lines (including Coster Kronig contributions, cascade effects).
- 4. Interpretation of spectra: Obtaining net intensities; artifacts.

TUESDAY PM

XRD

INTRODUCTION TO VOLUME H | Cotton Creek

Organizer & Instructor:

J.A. Kaduk, Illinois Institute of Technology, Naperville, IL, USA, jkaduk@iit.edu

A new volume of the International Tables for Crystallography, Volume H on powder diffraction is being prepared. This volume will include chapters on fundamental topics in powder diffraction, including specimen preparation, data processing, structure solution and refinement, and structure validation, as well as topical chapters on many different applications of powder diffraction. Volume H will be the first International Tables volume for which the on-line version should be considered the primary, and the print volume the secondary publication. The editors anticipate that the topical chapters will include raw data and instructions for processing, to help make Volume H the ultimate powder diffraction textbook. This workshop will detail the organization and content of the Volume, and provide a "sneak peek" at selected chapters.

MODELING & ANALYSIS OF SMALL-ANGLE SCATTERING—CONTINUED | Meadowbrook

Organizer & Instructors:

B. Landes, Dow Chemical Company, Midland, MI, USA, bglandes@dow.com

J. llavsky, Argonne National Laboratory, Argonne, IL, USA, ilavsky@aps.anl.gov

XRF

SAMPLE PREPARATION OF XRF | Standley Ballroom I

Organizer & Instructors:

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

J. Libal, Cliffs Natural Resources, Silver Bay, MN, USA

M. Bouchard, Corporation Scientifique Claisse, Quebec City, Quebec, Canada

This workshop will discuss fundamental physics and basic laboratory operations involved in the specimen preparation for XRF of pressed powders and fusion beads, with a special session devoted to the preparation of iron ore, concentrates and pellets.

QUANTITATIVE ANALYSIS—CONTINUED | Standley Ballroom II

Organizer & Instructors:

M. Mantler, Rigaku Corporation, Japan, michael.mantler@rigaku.com

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

B. Vrebos, PANalytical B.V, Almelo, The Netherlands

2013 ORAL SESSION

WEDNESDAY AM

PLENARY SESSION: THE 100TH ANNIVERSARY OF X-RAY SPECTROSCOPY | Standley Ballroom

Chair: G.J. Havrilla, Los Alamos National Laboratory, Los Alamos, NM, USA

9:00 CHAIRMAN OF THE DENVER X-RAY CONFERENCE OPENING REMARKS

W.Tim Elam, University of Washington APL, Seattle, WA, USA

PRESENTATION OF AWARDS

2013 BARRETT AWARD PRESENTATION

Recipient to be announced

2013 JENKINS AWARD PRESENTED TO RENE VAN GRIEKEN University of Antwerp, Antwerp, Belgium

Presented by W.Tim Elam, University of Washington APL, Seattle, WA, USA

2013 JEROME B. COHEN STUDENT AWARD The winner will be announced at the session.

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

2013 HANAWALT AWARD PRESENTED TO ROBERT B. VON DREELE Argonne National Laboratory, Lemont, IL, USA

Presented by Scott Misture, New York State College of Ceramics at Alfred University, Alfred, NY, USA

PLENARY SESSION REMARKS BY THE CHAIR

INVITED TALKS:

9:30 F-68 WDX: From Roentgen to Moseley to Bragg to Sherman to Jenkins

John A. Anzelmo, Anzelmo & Associates, Inc., Madison, WI, USA

10:15 BREAK

10:45 F72 THE ELECTRONIC AGE - EDX AND OTHER MODERN TECHNIQUES TO THE PRESENT AND BEYOND

Michael Mantler, Rigaku Corporation, Purkersdorf, Austria

11:30 D-74 Hanawalt Award Lecture: Protein Polycrystallography

Robert B. Von Dreele, Argonne National Laboratory, Lemont, IL, USA

WEDNESDAY PM

XRD & XRF

NEW DEVELOPMENTS IN XRD & XRF INSTRUMENTATION | Standley Ballroom I

Chairs: T. Fawcett, International Centre for Diffraction Data, Newtown Square, PA, USA, fawcett@icdd.com **T.N. Blanton**, Eastman Kodak Company Research Labs, Rochester, NY, USA, thomas.blanton@kodak.com

1:15 C-9 Real-time Monitoring of Process Stream Mineralogy and Elemental Composition with the XRDF System

J.N. O'Dwyer, J.R. Tickner, G.J. Roach, CSIRO, Sydney, NSW, Australia

1:30 C-12 REAL-TIME DUAL QUANTITATIVE ELEMENTAL AND MINERALOGICAL ANALYSIS OF GAS BEARING SHALE

T.C. Jennison, B. Boyer, W. Brunner, Olympus NDT, Campbell, CA, USA

WEDNESDAY PM CONTINUED

1:45 F-38 New Desktop Type XRF for On-Site Elemental Analysis

D. Matsunaga, K. Nishikata, T. Aoyama, S. Ohzawa, A. Kira, S. Komatani, HORIBA Ltd., Kyoto, Japan

2:00 F-I2 Trace Element Analysis in Geological, Coal, and Coke Samples Using EDXRF

J. Heckel, D. Sachtler, D. Wissmann, SPECTRO Analytical Instruments GmbH, Kleve, Germany M. Daniel-Prowse, M. DeLeon, SPECTRO Analytical Instruments Inc, Mahwah, NJ, USA

2:15 C-3 150 mm² Silicon Drift Detector Modules

A. Pahlke, M. Bachmann, T. Eggert, R. Fojt, M. Fraczek, L. Höllt, J. Knobloch, N. Miyakawa, S. Pahlke, J. Rumpff, O. Scheid, A. Simsek, R. Stötter, I. Wennemuth, F. Wiest, KETEK GmbH, Munich, Germany

2:30 C-14 THE NEXT GENERATION: HIGHSCORE PLUS V4.0

T. Degen, E. Bron, M. Sadki, PANalytical B.V., Almelo, The Netherlands

2:45 **B**REAK

3:15 D-58 THE INSIDE VIEW ON NANO-MATERIALS WITH THE XEUSS SAXS-WAXS SYSTEM

P. Panine, M. Fernandez-Martinez, S. Rodrigues, B. Lantz, R. Mahe, F. Bossan and P. Høghøj, Xenocs, Sassenage, France

3:30 D-30 THE N8 HORIZON FOR DEDICATED SAXS, WAXS, AND GISAXS

B. Jones, J. Giencke, B. He, H. Ress, Bruker AXS, Madison, WI, USA G. Vanhoyland, K. Erlacher, Bruker AXS, Karlsruhe, Germany

3:45 C-11 Moxtek's New 60 KV, 12W X-ray Source: Performance Characterizations

S. Cornaby, E. Miller, R. Steck, K. Kozaczek, S. Kamtekar, Moxtek, Orem, UT, USA

4:00 D-20 THE VERSATILITY OF THE INCOATEC MICROFOCUS SOURCE

B. Hasse, A. Kleine, J. Graf, J. Wiesmann, C. Michaelsen, Incoatec GmbH, Geesthacht, Germany

4:15 D-10 Low Cost Rolled X-ray Prism Lenses to Increase Photon Flux Density in Diffractometry Experiments

H.Vogt, A. Last, J. Mohr, F. Marschall, M. Kluge, V. Nazmov, Karlsruhe Institute of Technology (KIT) / Institute of Microstructure Technology, Karlsruhe, Baden-Württemberg, Germany

K.-U. Mettendorf, R. Eisenhower, Bruker AXS GmbH, Karlsruhe, Baden-Württemberg, Germany

4:30 D-18 A Novel X-ray Detector for In-House XRD

T.Taguchi, K. Matsushita, T. Sakumura, Y.Tsuji, T. Nagayoshi, Y. Nakaye, RIGAKU Corporation, Akishima, Tokyo, Japan

4:45 D-79 SCATTERX⁷⁸ - A HIGH-PERFORMANCE SAXS/WAXS MODULE INTEGRATED ON A MULTI-PURPOSE X-RAY DIFFRACTOMETER PLATFORM

J. Bolze, M. Fransen, PANalytical B.V., Almelo, The Netherlands

V. Kogan, DANNALAB B.V., Enschede, The Netherlands

XRD

HIGH ENERGY XRD || Cotton Creek

Chair: J. Almer, APS, Argonne National Laboratory, Argonne, IL, USA, almer@aps.anl.gov

1:30 D-75 Invited—High Energy X-ray Diffraction Microscopy: Direct Observation of 3D Materials Response

R.M. Suter, Carnegie Mellon University, Pittsburgh, PA, USA

WEDNESDAY PM CONTINUED

2:00 D-49 Invited—A New High Energy X-ray Station at the Cornell High Energy Synchrotron Source

M.P. Miller, B. Oswald, M. Koker, J. Brock, E. Fontes, Cornell High Energy Synchrotron Source, Ithaca, NY USA J. Schuren, Air Force Research Laboratory, Wright Patterson AFB, OH, USA P. Ko, Applied and Engineering Physics, Cornell University, Ithaca, NY, USA

2:30 D-46 In SITU CHARACTERIZATION OF GRADE 92 STEEL DURING TENSILE DEFORMATION USING HIGH ENERGY X-RAY DIFFRACTION AND SMALL ANGLE X-RAY SCATTERING

L. Wang, M. Li, J. Almer, Argonne National Laboratory, Lemont, IL, USA

2:50 D-48 Understanding Cyclic Plasticity and Fatigue Using High Energy X-ray Diffraction and Crystal-Based Finite Element Models

M. Obstalecki, S.L. Wong, P.R. Dawson, M.P. Miller, Cornell University, Ithaca, NY, USA

- 3:10 BREAK
- 3:30 D-77 Invited—A Combined Approach to Mapping Orientations, Strains, and Voids/Cracks/Inclusions During Loading Using High Energy X-rays

J.C. Schuren, AFRL, Wright-Patterson Air Force Base, OH, USA

4:00 D-67 DECOMPOSITION OF THE ALPHA"/BETA DUPLEX-PHASE MICROSTRUCTURE DURING CONTINUOUS HEATING OF A NEAR-BETA TITANIUM ALLOY

P. Barriobero-Vila, F. Warchomicka, G. Requena, Institute of Materials Science and Technology, Vienna University of Technology, Vienna, Austria

M. Stockinger, Böhler Schmiedetechnick GmbH & Co KG, Kapfenberg, Austria

N. Schell, A. Stark, Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

T. Buslaps, ID15, European Synchrotron Radiation Facility, Grenoble, France

4:20 D-47 Understanding SLIP Processes in Silicon Using High Energy X-rays

D.C. Pagan, M.P. Miller, Cornell University, Ithaca, NY, USA

XRF

QUANTITATIVE ANALYSIS || Standley Ballroom II

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

- 1:30 F-7 INVITED—QUANTITATIVE ANALYSIS OF AMBIENT AND SOURCE AIR FILTERS
 - S.D. Kohl, J.G Watson, J.C Chow, Desert Research Institute, Reno, NV, USA
- 2:00 F-17 Invited—Studies Using TXRF for Analysis of Aerosols Containing Nanoparticles with Designed Shapes and Those Produced From Fabric Testing

U.E.A. Fittschen, M. Menzel, L. Eggers, Institute of Inorganic and Applied Chemistry, University of Hamburg, Hamburg, Germany

2:30 F-59 Trace Analysis for Metals in Nail Polish by Wavelength Dispersive X-ray Fluorescence (WDXRF)

A.C. McWilliams, M.A. Levine, F.X. Weber, K.E. Levine, Research Triangle Institute, Research Triangle Park, NC, USA A.A. Martin, Thermo Fisher Scientific, Sugarland, TX, USA

2:50 F-15 REVISIT OF FORENSIC ANALYSIS OF ARSENIC POISONING CASE 1998

J. Kawai, Department of Materials Science and Engineering, Kyoto University, Kyoto, Japan

WEDNESDAY PM CONTINUED

- 3:10 BREAK
- 3:30 F-8 Invited—Evaluation of Fundamental Parameters for Quantitative X-ray Fluorescence of Polyolefins
 - D. Burns, M. Wright, S. Yusuf, Dow Chemical, Midland, MI, USA
- 4:00 F-39 COMPARISON OF CALCULATION METHODS FOR ANALYSIS OF SOIL SAMPLES
 M. Cameron, A. Seyfarth, Bruker, Kennewick, WA, USA
- 4:20 F-24 NECESSARY CONDITIONS FOR ROBUST FUNDAMENTAL PARAMETER ANALYSIS IN EDXRF T. Papp, J.A. Maxwell, Cambridge Scientific, Guelph, ON, Canada
- 4:40 F-22 Use of Surrogate Model Elements for Accurate Plutonium Quantification with HiRX
 - K.G. McIntosh, G.J. Havrilla, Los Alamos National Laboratory, Los Alamos, NM, USA

THURSDAY AM

XRD & XRF

- APPLICATIONS OF XRD & XRF IN THE PETROLEUM INDUSTRY | Standley Ballroom II
 - Chairs: A. Doyle, Pontifical Catholic University of Rio de Janeiro (PUC-Rio), Rio de Janeiro, Brazil, doyle@puc-rio.br D.E. Simon, DES Consulting, Bartlesville, OK, USA, desconsulting@sbcglobal.net R.W. Morton, Phillips 66, Bartlesville, OK, USA, bob.morton@p66.com
 - 9:00 F-3 INVITED—DETERMINATION OF CHLORINE IN CRUDE OIL BY ENERGY DISPERSIVE X-RAY FLUORESCENCE SPECTROMETRY
 - R.Q. Aucelio, A. Doyle, Pontifical Catholic University of Rio de Janeiro, Rio de Janeiro, Brazil
 - 9:30 F-34 BENEFITS USING WDXRF FOR PROCESS CONTROL IN POLYMER PRODUCTION: THE ACCURATE ANALYSIS OF IMPURITIES AND ADDITIVES IN PE AND PP
 - A. Buman, D. Pecard, Bruker AXS, Madison, WI, USA
 - K. Behrens, A. Bühler, F. Portala, Bruker GmbH, Karlsruhe, Germany
 - 9:50 F-60 ADVANCED GEOLOGICAL APPLICATIONS USING WDXRF ELEMENTAL MAPPING/SMALL SPOT ANALYSIS AND STANDARDLESS QUANTIFICATION
 - A. Martin, Thermo Fisher Scientific, Sugarland, TX, USA
 - D. Bonvin, K. Juchli, Thermo Fisher Scientific, Ecublens, Switzerland
 - A.C. McWilliams, Research Triangle Institute, Research Triangle Park, NC, USA
- 10:10 F-63 Invited—Some Applications of XRF in the Petroleum Industry
 - A. Saavedra, Petrobras, Rio de Janeiro, RJ, Brazil
- 10:40 BREAK
- II:00 D-72 Invited—Crystallite Domain Size and The Long-Range Order Index
 - R.W. Morton, Phillips 66 Company, Bartlesville, OK, USA
 - D.E. Simon, DES Consulting, Bartlesville, OK, USA
- 11:30 D-73 DETERMINATION OF BA/SR RATIO IN THE BARITE/CELESTITE SOLID SOLUTION SERIES
 - D.E. Simon, DES Consulting, Bartlesville, OK, USA
 - R.W. Morton, Phillips 66 Company, Bartlesville, OK, USA

THURSDAY AM CONTINUED

XRD

STRESS ANALYSIS || Cotton Creek

Chairs: D. Brown, Los Alamos National Laboratory, Los Alamos, NM, USA, dbrown@lanl.gov **T.R. Watkins**, Oak Ridge National Laboratory, Oak Ridge, TN, USA, watkinstr@ornl.gov

8:00 D-36 Invited—High-Energy X-ray Studies of Microstructure and Strain Evolution Under Thermo-Mechanical Deformation

J. Almer, P. Kensei, J. Okasinski, Argonne National Laboratory, Argonne, IL, USA

8:30 D-51 A METHOD TO MEASURE 3D RESIDUAL STRESS FIELDS USING HIGH ENERGY X-RAYS AND A FINITE ELEMENT DISCRETIZATION

M.P. Miller, P.R. Dawson, J.-S. Park, K. McNelis, Cornell University, Ithaca, NY, USA

U. Lienert, Deutsches Elektronen-Synchrotron, Hamburg, Germany

J.C. Williams, The Ohio State University, Columbus, OH, USA

8:50 D-65 DUCTILITY OF BERYLLIUM SUBJECTED TO SHEAR-COMPRESSION INVESTIGATED USING SYNCHROTRON X-RAY DIFFRACTION

T.A. Sisneros, D. Brown, B. Clausen, C. Cady, G.T. Gray III, E. Tulk, Los Alamos National Laboratory, Los Alamos, NM, USA

J.Almer, Argonne National Laboratory, Argonne, IL, USA

9:10 D-55 SPATIALLY RESOLVED RESIDUAL STRAINS AND STRESSES IN AS-FABRICATED NUCLEAR FUEL PLATES

M.A. Okuniewski, Idaho National Laboratory, Idaho Falls, ID, USA

D.W. Brown, E. Tulk, B. Clausen, L. Balogh, Los Alamos National Laboratory, Los Alamos, NM, USA J. Almer, J. Okasinski, Argonne National Laboratory, Argonne, IL, USA

9:30 D-11 Sub-Micronic Phase, Strain and Texture in Depth Gradient Measurement in Polycrystalline Thin Film: A Nano-Pencil Beam Diffraction Approach

N. Vaxelaire, P. Gergaud, CEA, LETI, Grenoble, France

G.B.M. Vaughan, European Synchrotron Radiation Facility, Grenoble, France

9:50 D-23 Phase Reversion during Compressive Loading of Shocked Alpha/Omega Zirconium

B. Clausen, Lujan Center, Los Alamos National Laboratory, Los Alamos, NM, USA

E.Tulk, E. Cerreta, J.P. Escobedo-Diaz, T.A. Sisneros, D.W. Brown, MST-8, Los Alamos National Laboratory, Los Alamos, NM, USA

J.Almer, Advanced Photon Source, Argonne National Laboratory, Argonne, IL, USA

10:10 BREAK

10:40 D-66 Invited—Grinding Burn - A Residual Stress Problem

B. Eigenmann, X-ray and Materials Laboratory Eigenmann, Schnaittach - Hormersdorf, Germany

11:10 D-13 THE GENERALIZED SIN²ψ METHOD: An Advanced Solution for X-ray Stress Analysis in Textured Materials

A. Haase, M. Klatt, A. Schafmeister, R. Stabenow, GE Sensing & Inspection Technologies GmbH, SEIFERT Analytical X-ray, Ahrensburg, Germany

B. Ortner, Montan Universität, Leoben, Austria

11:30 D-43 RESIDUAL STRESS AND QUANTITATIVE PHASE MAPPING ON COMPLEX GEOMETRIES

M. Allahkarami, J.C Hanan, Oklahoma State University, OK, USA

THURSDAY AM CONTINUED

PAIR DISTRIBUTION FUNCTION | Meadowbrook

Chair: L. Ehm, Stony Brook University—Mineral Physics Institute, Stony Brook, NY, USA and Brookhaven National Laboratory, Upton, NY, USA, lars.ehm@stonybrook.edu

9:00 D-22 Invited—Application of Pair Distribution Function Analysis in Environmental Nanoscience

F.M. Michel, Virginia Tech, Blacksburg, VA, USA

9:30 D-26 Invited—High Pressure Investigations of Liquid and Polymerized CO up to 20 GPa Using Pair Distribution Function Analysis

N. Rademacher, L. Bayarjargal, W. Morgenroth, B. Winkler, Goethe University, Frankfurt am Main, Germany J. Ciezak-Jenkins, S. Batyrev, US Army Research Laboratory, Aberdeen Proving Grounds, MD, USA

10:00 D-25 High Energy X-ray Powder Diffraction at Petra III – Real Space Data in Real Time Under Real Conditions

A.-C. Dippel, J. Torben Delitz, P. Walter, H.-P. Liermann, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

M. Hinterstein, Institut fuer Werkstoffwissenschaft, Technische Universität, Dresden, Germany

10:20 BREAK

10:50 D-15 Neutron Pair Distribution Function Study of Hydrogen Loaded Pu-Ga Alloys

A.I. Smith, K.L. Page, S. Richmond, J. Siewenie, T.A. Saleh, F. Hampel, M. Ramos, A. Llobet-Megias, J.N. Mitchell, D.S. Schwartz, Los Alamos National Laboratory, Los Alamos, NM, USA

11:10 D-81 Ambient and Variable-Temperature PDF Studies on a Laboratory Instrument

M. Sommariva, M. Gateshki, C.A. Reiss, M. Fransen, PANalytical B.V., Almelo, The Netherlands

XRF

APPLICATIONS FOR PORTABLE XRF | Standley Ballroom I

Chair: K.A. Russell, Olympus Innov-X, Woburn, MA, USA, kimberley.russell@olympusndt.com Co-Chair: W. Benzel, USGS, Denver, CO, USA

9:10 F-71 Invited—Use of Handheld XRF Analyses in the Characterization, Assessment, Remedial Design, and Cleanup of Lead Contaminated Sites in Developing Countries

I.H. von Lindern, TerraGraphics International Foundation, Moscow, Idaho, USA

9:40 F-41 Performance Comparison of Portable XRF Instruments: A Mineral Exploration Industry Prospective

N.W. Brand, C.J. Brand, Portable XRF Services Pty Ltd, West Perth, Australia

10:00 BREAK

10:30 F-4 RAPID SCREENING OF LIQUID DIETARY SUPPLEMENTS FOR NANOSCALE SILVER USING A PORTABLE X-RAY FLUORESCENCE ANALYZER (P-XRF)

G. Sanchez-Pomales, T. K. Mudalige, J.-H. Lim, S.W. Linder, U.S. Food and Drug Administration, Arkansas Regional Laboratory, Jefferson, AR, USA

THURSDAY AM CONTINUED

10:50 F-6 PORTABLE X-RAY FLUORESCENCE FOR SEED TREATMENT TECHNOLOGY

W.W. Brubaker, L. Zhang, M.J. Enderle, DuPont Corporate Center for Analytical Sciences, Wilmington, DE, USA P.T. Richardson, P. Stchur, S. Vanaman, C.A. Daly, S. Lumsdon, R.A. Kaczmarczyk, DuPont Crop Protection, Newark, DE, USA

I 1:10 F-37 THE ROLE OF HANDHELD XRF IN DELINEATING THE EXTENT AND DEGREE OF LEAD CONTAMINATION IN SOILS ASSOCIATED WITH ARTISANAL GOLD MINING, NORTHWESTERN NIGERIA

W.M. Benzel, G.S. Plumlee, U.S. Geological Survey, Denver, CO, USA

THURSDAY PM

XRD & XRF

APPLIED MATERIAL ANALYSIS || Cotton Creek

Chairs: T. Fawcett, International Centre for Diffraction Data, Newtown Square, PA, USA, fawcett@icdd.com **T.N. Blanton**, Eastman Kodak Company Research Labs, Rochester, NY, USA, thomas.blanton@kodak.com

- 1:00 D-57 INVITED—STRUCTURE DESIGN OF NEW CATHODE MATERIALS FOR LI-ION BATTERIES

 E.V.Antipov, N.R. Khasanova, O.A. Drozhzhin, Department of Chemistry, Moscow State University, Moscow, Russia
- I:30 D-38 IN-SITU MONITORING OF VANADIUM OXIDE FORMATION USING HIGH TEMPERATURE XRD M.A. Rodriguez, N.S. Bell, J.J.M. Griego, C. Edney, Sandia National Laboratories, Albuquerque, NM, USA
- 1:50 D-45 STRUCTURE DETERMINATION AND REFINEMENT OF HIGH SYMMETRIC LED PHOSPHOR MATERIALS USING XRD POWDER DIFFRACTION

Y.-i. Jang, K.-y. Hong, K.-h. Park, LG Electronics, Seoul, Korea

- 2:10 D-31 Macroscopic Metrology of Nanoscale Materials
 - J. Giencke, B. Jones, M. Sunder, H. Cordes, B. He, Bruker AXS, Madison, WI, USA
- 2:30 D-9 In Situ Observation of Liquid Sintering of Calcium-Ferrite by Quick X-ray Diffraction System
 - R. Murao, M. Kimura, Nippon Steel & Sumitomo Metal, Futtsu, Chiba, Japan
 - N. Ohta, Nippon Steel Technoresearch, Futtsu, Chiba, Japan
- 2:50 C-8 HAPG Mosaic Crystals and Their Application in High Resolution X-ray Spectroscopy

M. Gerlach, B. Beckhoff, I. Holfelder, Physikalisch-Technische Bundesanstalt, Berlin, Germany L. Anklamm, H. Legall, W. Malzer, C. Schlesiger, Technical University Berlin, Berlin, Germany

A. Antonov, I. Grigorieva, Optigraph GmbH, Berlin, Germany

- 3:10 BREAK
- 3:30 D-7 DIFFRACTION STUDIES OF SELECTED MOLECULAR SIEVES AND METAL ORGANIC FRAMEWORK MATERIALS FOR CO₂ CAPTURE APPLICATIONS

 $\textbf{W.Wong-Ng}, L. \ Espinal, A. \ Allen, Q. \ Huang, NIST, Gaithersburg, MD, USA$

J.A. Kaduk, Illinois Institute of Technology, Chicago, IL, USA

L. Li, Boise State University, Boise, ID, USA

M.R. Suchomel, Advanced Photon Source, Argonne National Laboratory, Argonne, IL, USA

THURSDAY PM CONTINUED

3:50 D-19 X-ray Investigations of Solid Solutions of Monocalciumaluminate and Monostrontiumaluminate Important Phases in Cement and Phosphorescence Materials

H. Pöllmann, University Halle, Halle, Germany

4:10 C-5 DEVELOPMENT OF GRATING-BASED STROBOSCOPIC X-RAY PHASE IMAGING USING POLYCHROMATIC LABORATORY AND SYNCHROTRON X-RAY SOURCES

M.P. Olbinado, The University of Tokyo, Kashiwa, Chiba, Japan

P. Vagovic, W. Yashiro, A. Momose, Tohoku University, Aoba, Sendai, Japan

4:30 C-2 CHARACTERIZATION OF MATERIALS USING COMBINED X-RAY MICROANALYSIS AND DIFFRACTION METHODS

S. Addepalli, T. Shalini, GE Global Research, Bangalore, Karnataka, India

4:50 D-8 MATERIALS CHARACTERIZATION FROM DIFFRACTION INTENSITY DISTRIBUTION IN GAMMA DIRECTION

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

XRD

POLYMERS || Meadowbrook

Chair: L. Liu, Beijing Research Institute of Chemistry, Beijing, China, violetlj208@gmail.com

1:30 D-41 Invited—USAXS/SAXS/WAXS Instrument for Materials Research

J. Ilavsky, P.R. Jemian, G.G.Long, Advanced Photon Source, Argonne National Laboratory, Argonne, IL, USA A.J. Allen, F. Zhang, L.E. Levine, National Institute of Standards and Technology, Gaithersburg, MD, USA

2:15 D-42 ORIENTATION, CRYSTALLINITY, AND MECHANICAL PROPERTIES OF BIAXIALLY STRETCHED POLYETHYLENE TEREPHTHALATE FILMS USING X-RAY DIFFRACTION

S. Bandla, M. Allahkarami, J.C. Hanan, Oklahoma State University, Tulsa, OK, USA

2:45 D-34 A New "Chain" of Events: Polymers in the Powder Diffraction File™ (PDF®)

S.D. Gates, S.N. Kabekkodu, T.G. Fawcett, International Centre for Diffraction Data, Newtown Square, PA, USA T.N. Blanton, Eastman Kodak Company Research Labs, Rochester, NY, USA J.A. Kaduk, Illinois Institute of Technology, Chicago, IL, USA

3:15 BREAK

3:45 D-2 CHARACTERIZING PROCESS INDUCED CRYSTAL MODIFICATIONS IN POLY(ETHERKETONEKETONE) (PEKK) BY SCATTERING TECHNIQUES

P. Ricou, B. Clay, Arkema Inc., King of Prussia, PA, USA M. Garcia-Leiner, Exponent, Bowie, MD, USA

4:15 D-6 X-RAY SCATTERING ON CASEIN MICELLES AND HIGH DENSITY LIPOPROTEIN (HDL) GRANULES DURING PROCESSING OF FOODS

R. Gebhardt, Technische Universität München, Freising, Bavaria, Germany

THURSDAY PM CONTINUED

XRF

FUSION & INDUSTRIAL APPLICATIONS OF XRF || Standley Ballroom I

Chair: J.A. Anzelmo, Anzelmo & Associates, Inc., Madison, WI, USA, jaanzelmo@aol.com Co-chair: J.V.Thomas, Wyoming Analytical Labs, Laramie, WY, USA, jthomas@wal-lab.com

1:30 F-67 Invited—Application of XRF to Combustion Residues

J.V.Thomas, C.R.Wilson, Wyoming Analytical Laboratories, Inc., Laramie, WY, USA

2:00 F-53 MERCURY EMISSIONS MONITORING BY TXRF

M. Garcia, N. Kumar, nanoXRF, Fort Worth, TX, USA

2:20 F-51 HIGH-PRECISION ANALYSIS OF IRON ORE BY WAVELENGTH-DISPERSIVE X-RAY FLUORESCENCE SPECTROMETRY

B. Vrebos, PANalytical, Almelo, The Netherlands

2:40 F-20 ISO 9615-1 SIMPLIFIED BORATE FUSION / WDXRF ANALYTICAL METHOD FOR IRON ORE INCLUDING TOTAL IRON ANALYSIS: PART 2

M. Bouchard, A. Milliard, S. Rivard, Claisse, Corporation Scientifique, Québec, QC, Canada

S. Ness, Intertek Genalysis, Perth, Australia

3:00 BREAK

3:30 F-19 THE STUDY OF CHLORINE ANALYSIS BY XRF USING SAMPLE PREPARATION BY BORATE FUSION FOR CEMENT INDUSTRY RELATED MATERIALS

M. Bouchard, A. Milliard, S. Rivard, Claisse, Corporation Scientifique, Québec, QC, Canada

3:50 F-29 Aerosol Filter Analysis Using Polarized Optics EDXRF with Thin Film FP Method

A. Morikawa, T. Moriyama, M. Doui, Rigaku Corporation, Osaka, Japan

S. Fess, Applied Rigaku Technologies, Inc., Austin, TX, USA

4:10 F-40 Extremely High Count-Rate Performance of Silicon Drift Detector

S. Barkan, L. Feng, V. D. Saveliev, M. Takahashi, Y. Wang, M. Uehara, E. V. Damron, Hitachi High-Technologies Science America, Inc., Northridge, CA, USA

MICRO XRF || Standley Ballroom II

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

1:50 F-61 Invited—Superconducting Microcalorimeters for Time-Resolved and Other Photon-Starved X-ray Spectroscopies

J. Uhlig, J. Ullom, W.B. Doriese, J. Fowler, C. Reintsema, D. Swetz, D. Bennett, G. Hilton, K. Irwin, D. Schmidt, NIST Boulder, Boulder, CO, USA

J. Uhlig, W. Fullagar, N. Gador, S. Canton, K. Kinnunen, V. Sundstrom, Lund University Chemical Physics, Lund, Sweden

2:20 F-11 CHARACTERIZATION OF METAL DOPED POLYMER CAPSULES USING CONFOCAL MICRO X-RAY FLUORESCENCE SPECTROSCOPY AND X-RAY COMPUTED TOMOGRAPHY

N.L. Cordes, G.J. Havrilla, K.A. Obrey, B.M. Patterson, Los Alamos National Laboratory, Los Alamos, NM, USA

THURSDAY PM CONTINUED

2:40 F-69 Invited—High Resolution X-ray Fluorescence Microscopy: Challenges and Opportunities

S. Vogt, C. Jacobsen, Argonne National Laboratory, Argonne, IL, USA and Northwestern University, Evanston, IL, USA S. Chen, S.-C. Gleber, L. Finney, J. Ward, D. Vine, L. Trahey, J. Maser, B. Lai, Argonne National Laboratory, Argonne, IL, USA

- J. Deng, R. Mak, T. Paunesku, K. Brister, G. Woloschak, Northwestern University, Evanston, IL, USA
- L. Makowski, Northeastern University, Boston, MA, USA
- C. Flachenecker, Xradia Inc., Pleasanton, CA, USA
- 3:10 BREAK
- 3:40 F-44 Invited—Confocal MicroXRF in Vacuum: Setup and Applications
 - C. Streli, S. Smolek, B. Pemmer, P. Wobrauschek, Atominstitut, Vienna, Austria
- 4:10 F-21 MICRO X-RAY FLUORESCENCE IN FOOD FORENSICS & FOOD SAFETY
 - V.L. St. Jeor, Cargill Incorporated, Excelsior, MN, USA
- 4:30 F-14 FORENSIC APPLICATION OF MICRO-XRF: DETERMINATION OF UNIQUE COMPOSITIONAL PATTERNS IN GLASSES: MULTIVARIATE APPROACH AND STATISTICAL ANALYSIS
 - S. Mamedov, Horiba Scientific, Edison, NJ, USA
- 4:50 F-50 THICKNESS AND COMPOSITION ANALYSIS OF THIN-FILM SOLAR CELLS VIA MICRO-XRF A. Lee, M. Chipman, B. Scruggs, EDAX, Mahwah, NJ, USA

FRIDAY AM

XRD

NEW DEVELOPMENTS IN RIETVELD ANALYSIS || Standley Ballroom II

Chair: M. Suchomel, APS - Argonne National Laboratory, Lemont, IL, USA, suchomel@aps.anl.gov

8:30 D-32 Invited—Representational Analysis of Extended Disorder in Large Atomistic Ensembles Generated from Diffraction Data

J.R. Neilson, Colorado State University, Fort Collins, CO, USA

T.M. McQueen, Johns Hopkins University, Baltimore, MD, USA

9:00 D-4 STRUCTURAL STUDY OF NANOSTRUCTURED CR-CO BASED ALLOYS BY X-RAY DIFFRACTION LINE PROFILE ANALYSIS

- S. Louidi, Université 20 Août 1955, Skikda, Algérie
- F.Z. Bentayeb, Université Badji-Mokhtar, Annaba, Algérie
- J.J. Sunol, L. Escoda, Universitat de Girona, Girona, Spain

9:20 D-62 A REAL SPACE RIGID BODY APPROACH TO QUANTIFYING INCOMMENSURATE STACKING FAULTS IN LAYERED OXIDES

- S.T. Misture, Alfred University, Alfred, NY, USA
- 9:40 BREAK

10:00 D-60 Invited—Combining Powder Diffraction with Solid State NMR Spectroscopy for Structure Elucidation via Rietveld Analysis

- M. Allix, F. Fayon, E. Véron, A.-L. Rollet, S. Cadars, G. Matzen, D. Massiot, Université d'Orléans, Orléans, France
- M. Suchomel, Argonne National Laboratory, Advanced Photon Source, Argonne, IL, USA
- F. Porcher, CEA Saclay, Gif Sur Yvette, France
- C. Martineau, Université de Versailles Saint-Quentin en Yvelines, Versailles, France

FRIDAY AM CONTINUED

10:30 D-29 CRYSTAL STRUCTURES OF SRR2SC2O7, R = PR, ND, SM, EU, AND GD

J.A. Kaduk, Illinois Institute of Technology, Chicago, IL, USA W. Wong-Ng, NIST, Gaithersburg, MD, USA

10:50 D-54 IN SITU XRD STUDIES OF PDZN METHANOL STEAM REFORMING CATALYST

E.J. Peterson, J.A. Paiz, T. Hough, A. DeLaRiva, A.K. Datye, The University of New Mexico, Albuquerque, NM, USA

XRF

TRACE ANALYSIS || Standley Ballroom I

Chair: M.A. Zaitz, IBM, Hopewell Junction, NY, USA, zaitz@us.ibm.com

8:30 F-70 INVITED—GIXRF AND GIXAS AT TRACE LEVELS

F. Meirer, Fondazione Bruno Kessler, Povo (Trento), Italy and Utrecht University, Utrecht, The Netherlands

G. Pepponi, Fondazione Bruno Kessler, Povo (Trento), Italy

D. Ingerle, C. Streli, Atominstitut, Vienna University of Technology, Vienna, Austria

A. Mehta, P. Pianetta, Stanford Synchrotron Radiation Lightsource, Menlo Park, CA, USA

9:00 C-7 INVITED—THE HARD X-RAY MICRO/NANO-PROBE BEAMLINE P06 AT PETRA III/DESY: THE FIRST YEAR OF USER OPERATION

G. Falkenberg, DESY, Hamburg, Germany

9:30 F-58 ULTRA HIGH ENERGY X-RAY FLUORESCENCE DIRECT DETECTION OF PLUTONIUM AND URANIUM THROUGH CONTAINER WALLS

G.J. Havrilla, V.M. Montoya, K. McIntosh, Los Alamos National Laboratory, Los Alamos, NM, USA

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

D. Robinson, Argonne National Laboratory, Argonne, IL, USA

9:50 F-35 XRS FOR PREVENTIVE CONSERVATION IN EUROPEAN MUSEUMS

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

10:10 BREAK

10:30 F-43 HEAVY METAL ANALYSIS IN LENS AND AQUEOUS HUMOR OF CATARACT PATIENTS BY TOTAL REFLECTION X-RAY FLUORESCENCE SPECTROMETRY

M. Schmeling, Loyola University Chicago, Chicago, IL, USA

B.I. Gaynes, S. Tidow-Kebritchi, Stritch School of Medicine, Loyola University Chicago, Maywood, IL, USA

10:50 F-64 Use of X-ray Spectroscopy for Elemental Analysis of Complex Biological Samples

A. Pejovic-Milic, E. Da Silva, B. Kirkam, Ryerson University, Toronto, ON, Canada

11:10 F-42 Application of Total Reflection X-ray Fluorescence Spectrometry and Grazing Incidence X-ray Fluorescence to Genesis Solar Wind Samples

M. Schmeling, Loyola University Chicago, Chicago, IL, USA

Y. Choi, P.J. Eng, J.E. Stubbs, GSECARS University of Chicago, Argonne, IL, USA

I.V. Veryovkin, Argonne National Laboratory, Argonne, IL, USA

11:30 F-26 MICROANALYSIS OF RARE EARTH ELEMENTS USING PYROELECTRIC CRYSTAL

S. Imashuku, A. Imanishi, K. Ohira, J. Kawai, Kyoto University, Kyoto, Japan

PDF-4/Organics 2013

What's in your sample?

Verify your results with PDF-4/Organics

A comprehensive materials database featuring 471,257 organic and organometallic compounds.



Designed for rapid materials identification

Polymorph screening

Quality control

Drug & Excipients identification

Formulation analysis

Quantitative analysis

Polymorph identification

Crystallite size

COMPREHENSIVE STANDARDIZED QUALITY REVIEWED





www.icdd.com | marketing @icdd.com 610.325.9814 | toll-free 866.378.9331

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







(U.S. & Canada)

CAMBRIDGE

Distinguished Titles from Cambridge

E-books Available for most titles!

Introduction to Computational Materials Science Fundamentals to Applications Richard LeSar

427 pp. 339 b/w illus. 15 tables Hb: 978-0-521-84587-8: Price: \$95.00

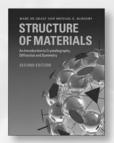


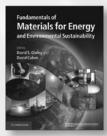
Second Edition!

Structure of Materials
An Introduction to Crystallography,
Diffraction and Symmetry

Marc De Graef and Michael E. McHenry

767 pp. 411 b/w illus. 90 tables 96 exercises Hb: 978-1-107-00587-7: Price: \$115.00





Fundamentals of Materials for Energy and Environmental Sustainability

Edited by
David S. Ginley and
David Cahen

772 pp. 450 color illus. 80 tables Hb: 978-1-107-00023-0: Price: \$99.00



Scanning Electron Microscopy for the Life Sciences

Edited by Heide Schatten

274 pp. 90 b/w illus. 39 color illus. Hb: 978-0-521-19599-7: Price: \$120.00



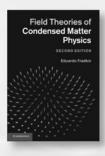
539 pp. 225 b/w illus. 25 tables Hb: 978-1-107-02375-8: Price: \$115.00

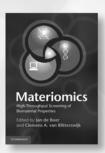


Second Edition!

Field Theories of Condensed Matter Physics Eduardo Fradkin

852 pp. 113 b/w illus. Hb: 978-0-521-76444-5: Price: \$99.00



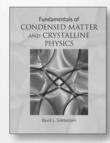


Materiomics

High-Throughput Screening of Biomaterial Properties

Edited by
Jan de Boer and
Clemens A. van Blitterswijk

219 pp. 60 b/w illus. Hb: 978-1-107-01677-4: Price: \$125.00



Fundamentals of Condensed Matter and Crystalline Physics

An Introduction for Students of Physics and Materials Science

David L. Sidebottom

418 pp. 229 b/w illus. 10 tables 95 exercises Hb: 978-1-107-01710-8: Price: \$75.00

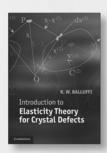
View all 2013 Engineering Catalogs at www.cambridge.org/us/engineering

Prices subject to change.

Introduction to Elasticity Theory for Crystal Defects

R. W. Balluffi

458 pp. 139 b/w illus. 3 tables 66 exercises Hb: 978-1-107-01255-4: Price: \$110.00



www.cambridge.org/engineering
@CambUP_engineer
800.872.7423 (North America)
+44 1223 326050 (Europe, Middle East, and Africa)



International Centre for Diffraction Data

Let our team of experts help you take your skills to the next level!

Fundamentals of X-ray Powder Diffraction: 3-7 June 2013



For the novice with some XRD knowledge or for the experienced with an interest in the theory behind XRD, this clinic offers a strong base for increased lab performance.

Covering instrumentation, specimen preparation, data acquisition and qualitative phase analysis. Handson use of personal computers for demonstration of the latest software; data mining with the PDF. The powder diffractometer: optical arrangement, factors affecting instrumental profile width, choice and function of divergence slit, calibration and alignment, detectors, X-ray optics.

*Advanced Methods in X-ray Powder Diffraction: 10-14 June 2013

For the experienced XRD scientist, this session offers enhanced analysis skills through intense problem solving, as well as an introduction to the Rietveld Method. Emphasizing computer-based methods of data collection and interpretation, both for qualitative and quantitative phase analysis.

Factors affecting d-spacing of crystals: unit cell, crystal structure, and solid solutions. Factors affecting diffraction-line intensities: relative and absolute intensities; structure-sensitive properties (atomic scattering and structure factors), polarization effects, and multiplicity; specimen-sensitive effects (orientation, particle size), measurement-sensitive effects (use of peak heights and peak areas), and choice of scanning conditions.

*Rietveld Refinement & Indexing Workshops:



Basic: 30 September-2 October 2013

Advanced: 3-4 October 2013

These completely hands-on computerized problem-solving workshops provide training in the use of the Rietveld method for crystal structure refinement.

Handheld XRF Workshop: 15-17 October 2013



The combination of portability, nondestructive on-site analysis, and relatively low cost has led to explosive growth in the use of handheld X-ray fluorescence spectrometers. This workshop will focus on XRF theory, X-ray safety, methods to optimize results, as well as various applications.

Practical X-ray Fluorescence: 28 April-2 May 2014



From theory to hands-on exercises, this course offers techniques and skills to improve lab performance. Discover the latest in cutting-edge instruments such as TXRF, hand-held devices, energy dispersive and wavelength dispersive spectrometers through live demonstrations.

The XRF course covers the basics of X-ray spectra; instrumentation design; methods of qualitative and quantitative analysis; specimen preparation and applications for both wavelength and energy dispersive spectrometry. Emphasizing quantitative methods; use of automated X-ray spectrometers; review of mathematical matrix correction procedures and new developments in XRF. Submit your samples for analysis by the XRF experts. Selected results will be the basis for class discussion!

* See the ICDD web site for prerequisites for advanced courses.

Location

ICDD Headquarters: 12 Campus Boulevard ◆ Newtown Square, Pennsylvania, 19073-3273 U.S.A.

For More Information

Contact Eileen Jennings, Education Coordinator

Tel: 610.325.9814 ♦ Fax: 610.325.9823 ♦ Email: clinics@icdd.com

Don't miss the opportunity to meet with our faculty, offering knowledge in a wide range of industries and applications. You'll meet seasoned professionals with experience in metals, microelectronics, thin films, indexing, polymers, organic chemistry and much more. Featuring live instruments for the XRF & XRD Clinics!



ICDD and the ICDD logo are registered in the U.S. Patent and Trademark Office.

2013-2014 Education Events

The Powder Diffraction File Difference

ICDD databases are the only crystallographic databases in the world with quality marks and quality review processes that are ISO certified.

The Powder Diffraction File

PDF-2 Release 2012 250,182 material entries PDF-4+ 2012 328,660 material entries WebPDF-4+ 2012 328,660 material entries PDF-4/Minerals 2012 39,410 material entries PDF-4/Organics 2013 471,257 material entries

Release 2012 of the Powder Diffraction File (PDF) contains 760,019 unique material entries.

> 760,019 **Entries**

Featuring

Standardized data 2002

Comprehensive coverage

Each data set is evaluated for quality

Designed for material identification and characterization

Data are reviewed, edited and corrected prior to publication

COMPREHENSIVE ❖ STANDARDIZED ❖ QUALITY REVIEWED





www.icdd.com | marketing@icdd.com 610.325.9814 | toll-free 866.378.9331 U.S. & Canada



2012

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







X'PERT POWDER

Your solution for powder analysis and more



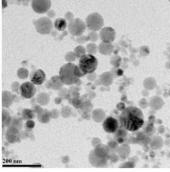


Versatile and easy to use

The basic configuration enables powder analysis by phase identification and quantification.

With easy and affordable extensions you can also:

- Analyze thin films
- Determine nanoparticle size distributions
- Investigate temperaturedependent material properties
- Perform automated analyses of multiple samples
- Benefit from the latest developments on optics, sample stages, detectors, X-ray tubes and analysis software





State-of-the-art performance for an attractive price

- · High-speed, high-quality data acquisition
- Up to five times faster than a benchtop system
 Multiple options for additional applications
- Automatic sample changer available
- Comprehensive and easy-to-use software
- More than 10 years of proven quality

Community of over 2500 user sites

Contact your local PANalytical sales representative.

info@panalytical.com www.panalytical.com



The Analytical X-ray Company



EQUINOX 100: A remarkable desktop x-ray diffractometer designed to out perform all others



Complete diffraction pattern in seconds

Simultaneous, real time measurement of the entire 2 theta range at high resolution

Ultra high brilliance x-ray source with focusing optic technology

Plugs into standard 110V outlet

No external cooling water supply necessary

No moving parts!

Reflection or transmission mode

Phase identification and quantification, Rietveld analysis

Equinox 100: Designed for QA applications and routine x-ray diffraction studies. Suitable for research in fields such as chemical, environmental, metallurgical, geological, cement, mining and pharmaceuticals



North America: (603)778-9161 • info@inel.us • www.inel.us
Headquarters in France: (33)2 38804545 • info@inel.fr • www.inel.fr

2013-2014 ICDD X-RAY CLINICS & WORKSHOPS

Practical XRF & XRD Training by the Industry's **Leading Experts!**

Sponsored by the

International Centre for **Diffraction Data**

Live Instrumentation Hands-on Training Theoretical Lectures

Fundamentals of X-ray Powder Diffraction—XRD I

3-7 June 2013

Advanced Methods in X-ray Powder Diffraction—XRD II 10-14 June 2013

Rietveld Refinement & Indexing:

Basic Workshop 30 September-2 October 2013 3-4 October 2013 **Advanced Workshop**

15-17 October 2013 **Handheld XRF Workshop**

Practical X-ray Fluorescence Spectrometry

28 April-2 May 2014

Register today at: www.icdd.com/education Email: clinics@icdd.com

Tel: 610.325.9814 Toll-free: (U.S. & Canada) 866.378.9331

ICDD and the ICDD logo are registered in the U.S. Patent and Trademark Office.





D8 DISCOVER with DAVINCI ULTRA GID:

The ultimate thin film characterization system.

- Push-button, motorized switching between in-plane and out-of-plane geometry
- In-plane grazing incidence diffraction (IP-GID) using full line-focus
- 100 times higher intensity than traditional methods
- Easy access to the full range of thin film XRD applications

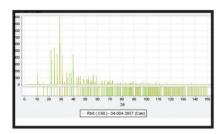
Contact us for more details and a system demonstration! www.bruker.com/d8discover

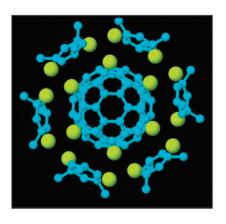
XRD



Designed for phase identification and quantitative analysis

Comprehensive materials database featuring 328,660 entries





- All entries have digital patterns for use in total pattern analysis
- 171,856 entries with atomic coordinates
- 45,286 entries with cross-referenced atomic coordinates
- 232,376 entries have I/I_c values for quantitative analysis by Reference Intensity Ratio
- All entries are stored in a standardized format for easy search and interpretation
- All entries go through a rigorous editorial process to ensure quality

COMPREHENSIVE ❖ STANDARDIZED ❖ QUALITY REVIEWED

www.icdd.com | marketing@icdd.com 610.325.9814 | toll-free 866.378.9331

(U.S. & Canada)











