

2013 DXC Summary

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LOCATION, DATES & ATTENDANCE

The 62nd Annual Denver X-ray Conference (DXC) was held in Westminster, Colorado at the Westin Hotel from 5 to 9 August 2013. The meeting attracted close to 300 registered attendees and well over 100 exhibit staff, all gathering to discuss applications, state-of-the-art techniques, and future developments in X-ray analysis. Thirty-one percent of the attendees were from outside the United States representing the following countries: Algeria, Australia, Austria, Belgium, Brazil, Canada, China, Croatia, the Czech Republic, France, Germany, Japan, Korea, Mexico, Russia, Sweden, The Netherlands, the United Kingdom and Venezuela. Thank you very much to those attendees and exhibitors who traveled a great distance so that we could all share a wonderfully unique international experience.

WORKSHOPS

Sixteen half-day tutorial workshops were held on Monday and Tuesday, with participation from 35 instructors. Various subjects were covered to satisfy the needs of both the beginner and the advanced attendee. Topics included:

XRD

- Introduction to the new GSAS-II Crystallographic Analysis System (full day)
- Basic to Intermediate XRD Analysis
- Total Pattern Analysis
- Hands-on Rietveld Analysis
- Modeling & Analysis of Small-angle Scattering (full day)
- Introduction to Volume H

XRF

- Basic XRF
- Trace Analysis
- Energy Dispersive XRF
- Quantitative Analysis (full day)
- Sample Preparation of XRF

Joint XRD & XRF

- X-ray Optics
- Fundamentals of Digital Signal Processing and X-ray Detectors

The instructors were a mix of leaders in industry, government and academia who graciously volunteered to work with the attendees and answer their questions. We thank the instructors for their valuable time.

SESSIONS

Nearly two-hundred presentations were made during the oral and poster sessions at DXC. Poster sessions were held on Monday and Tuesday evening in conjunction with evening receptions. XRD posters were displayed on Monday and XRF posters were shown on Tuesday. Each evening offered the authors a full two hours to show their work and network with their peers.

Thirteen half-day oral sessions were held on Wednesday afternoon, Thursday, and Friday morning. Session Chairs were experts in their respective field of X-ray analysis, and enhanced the program by inviting cutting-edge speakers to kick off their sessions. Session topics included:

Joint XRD & XRF

- New Developments in XRD & XRF Instrumentation
- Applications of XRD & XRF in the Petroleum Industry
- Applied Materials Analysis

XRD

- High Energy XRD
- Stress Analysis
- Pair Distribution Function
- Polymers
- New Developments in Rietveld Analysis

XRF

- Quantitative Analysis
- Applications for Portable XRF
- Fusion & Industrial Applications of XRF
- Micro XRF
- Trace Analysis

PLENARY SESSION AWARDS

Three awards were presented during the Plenary session. The *2013 Barrett Award* was presented to Vaclav Petricek of the Institute of Physics, Academy of Sciences of the Czech Republic, Praha, the Czech Republic. Dr Petricek received the award for “developing the theory of incommensurate/modulated/composite crystal structures and its implementation in the computing system Jana2006 (the most widely-used system for solving and refining aperiodic structures), and for making possible the correct archival of such structures in the Powder Diffraction FileTM”.

The *2013 Jenkins Award* was presented to Rene Van Grieken of the University of Antwerp, Antwerp, Belgium. Dr Van Grieken received the award for “contributions to the development and application of X-ray methods to a wide variety of topics, from aerosols in the environment to conservation and from new techniques and microanalysis to



biomedical applications. He has been a leader in the X-ray community and has served it in many capacities over the years, including Editor-in-Chief of *X-ray Spectrometry* as well as being a member of various national and international commissions involved in analytical and environmental chemistry. He has disseminated his knowledge in an impressive list of papers, books, and invited lectures”.

The 2013 Hanawalt Award was presented to Robert B. Von Dreele of Argonne National Laboratory, Lemont, IL, USA. Dr Von Dreele received the award for “his insight, courage and creativity in bringing powder diffraction to the macromolecular community”. Dr Von Dreele’s research focuses on the development of X-ray and neutron powder diffraction, and its application to a wide variety of scientific problems. He pioneered the General Structure Analysis System program suite for Rietveld analysis, a valuable method for structural analysis of nearly all classes of crystalline materials not available as single crystals. Currently, his work centers on further extensions of protein powder diffraction including investigation of crystal growth, phase transformations, radiation damage and exploring possible routes to *de novo* protein structure determination from powder data.

PLENARY – THE 100th ANNIVERSARY OF X-RAY SPECTROSCOPY

The Plenary Session, The 100th Anniversary of X-ray Spectroscopy, was held on Wednesday morning and chaired by George J. Havrilla of Los Alamos National Laboratory, Los Alamos, NM, USA. The history of X-ray Spectroscopy was celebrated and the pioneers of the technique were remembered and honored.

John A. Anzelmo of Anzelmo & Associates, Inc., Madison, WI, USA, gave the first invited talk, “WDX:

From Roentgen to Moseley to Bragg to Sherman to Jenkins” highlighting the foundation for X-ray Spectroscopy and major developments of the method. The second invited talk was given by Michael Mantler of the Rigaku Corporation, Purkersdorf, Austria. Dr Mantler spoke on, “The Electronic Age – EDX and Other Modern Techniques to the Present and Beyond”. His talk focused on current uses of X-ray Spectroscopy and how the practice will develop in the future.

In addition, Robert B. Von Dreele, Argonne National Laboratory, Lemont, IL, USA, presented the Hanawalt Award Lecture on “Protein Polycrystallography”. The presentation was given as part of the work that earned him the ICDD’s 2013 Hanawalt Award, which is presented every 3 years for an important, recent contribution to the field of powder diffraction.

ROBERT L. SNYDER STUDENT TRAVEL AWARD

The Robert L. Snyder Student Travel Awards offers travel support to enable graduate and undergraduate students to attend the Denver X-ray Conference. Six students received an award based on the relevancy and strength of their DXC presentation:

- Waleed Abuhani, Institute of Physics and Mathematics, Universidad Michoacána of San Nicolás de Hidalgo, Morelia, Michoacán, Mexico
Characterizing Fundamental Parameters Based Analysis for Soil-Ceramic Matrices in Polarized Energy Dispersive X-ray Fluorescence Spectrometry (pEDXRF)
- Magnus Menzel, University of Hamburg, Hamburg, Germany
Absorption of the Primary Beam in Sr-TXRF Analysis: Experimental Visualization Using a Color X-ray Camera

- Nadine Rademacher, Goethe University, Frankfurt am Main, Germany
High Pressure Investigations of Liquid and Polymerized CO up to 20 GPa Using Pair Distribution Function Analysis
- Sofiane Louidi, Université of 20 Août 1955, Skikda, Algeria
Structural Study of Nanostructured Cr-Co Based Alloys by X-ray Diffraction Line Profile Analysis
- Sudheer Bandla, Oklahoma State University, Tulsa, OK, USA
Orientation, Crystallinity, and Mechanical Properties of Biaxially Stretched Polyethylene Terephthalate Films using X-ray Diffraction
- Jiawanjun Shi, Alfred University, Alfred, NY, USA
Crystal Structure and Photocatalytic Studies of 2, 3, 4, and 5-Layer Aurivillius Oxides

BEST POSTER AWARDS

The awards were named on Monday and Tuesday evening at the end of the XRD and XRF poster sessions. The following posters won the awards:

XRD Best Poster Awards:

- An *in-situ* XRD and H₂-D₂ Exchange Study on Ni-Based Amorphous and Crystalline Membranes
A. Adibhatla, W. Chien, D. Chandra, University of Nevada, Reno, NV, USA
M.D. Dolan, CSIRO Energy Technology, Pullenvale, Queensland, Australia.
- Simulating X-ray Diffraction Profiles of Nanomaterials
H. Öztürk, I.C. Noyan, Columbia University, New York, NY, USA
H. Yan, NSLS II, Brookhaven National Laboratory, Upton, NY, USA.
- X-ray Diffraction Characterization of a Distorted Debye-Scherrer Film Strip – The Effect of Deacetylation on Cellulose Triacetate and an Improved Structural Model for Cellulose II
T.N. Blanton, International Centre for Diffraction Data, Newtown Square, PA, USA
J.A. Kaduk, Illinois Institute of Technology, Chicago, IL, USA
Q. Johnson, Materials Data Incorporated, Livermore, CA, USA.

XRF Best Poster Awards

- Investigation on the Ni Oxidation State in LiNi_{0.5}Mn_{1.5}O₄ Li-Ion Battery Cathodes at Different Cycle States: Pristine, Discharged, After Quick Charging and Slow Charging
U.E.A. Fittschen, M. Menzel, A. Schlifke, M. Froeba, Chemistry Department, University of Hamburg, Hamburg, Germany
U. Boesenberg, DESY Deutsches Elektronen Synchrotron, Hamburg, Germany
M. Falk, J. Janeck, Chemistry Department, University of Giessen, Giessen, Germany.
- Forensic Investigations with Different Confocal Micro-XRF Spectrometers

- S. Smolek, C. Strelj, P. Wobrauschek, Vienna Univ. of Technology, Atominstut, Vienna, Austria
- T. Nakazawa, K. Nakano, K. Tsuji, Osaka City University, Sumiyoshi, Osaka, Japan.
- Fast Elemental Imaging by Wavelength Dispersive X-ray Fluorescence Imaging Spectrometer
T. Ohmori, S. Emoto, Osaka City University, Osaka, Japan
S. Kato, M. Doi, T. Shoji, Rigaku Co., Takatsuki, Osaka, Japan
K. Tsuji, Osaka City University, Osaka, Japan.

EXHIBITS

Thirty-eight companies exhibited at the conference, displaying various products and services for X-ray diffraction and X-ray fluorescence. The countries represented were Canada, Germany, Japan and the United Kingdom. Companies participating as exhibitors were:

AMPTEK, Inc.
Angstrom, Inc.
Blake Industries, Inc.
Bruker AXS
Cambridge University Press
Chemplex Industries, Inc.
Claisse, Corporation Scientifique
Herzog Automation Corp.
Hitachi High-Technologies Science America, Inc.
HORIBA Scientific
Huber Diffraction GmbH/AXO Dresden
IFG – Institute for Scientific Instruments GMBH
Incoatec GmbH
Inel, Inc
International Centre for Diffraction Data
KETEK
labZY
Materials Data, Inc.
Materion Electrofusion
Micromatter
Mikron Digital Instruments, Inc.
Mineral Stats, Inc.
MOXTEK, Inc.
nanoXRF
Navas Instruments
Olympus
PANalytical
Premier Lab Supply
Proto Manufacturing
Rigaku Americas Corp.
Rigaku Innovative Tech
SGX Sensortech (MA) Ltd
Spectro Analytical Instruments
SPEX Sample Prep
Thermo Scientific
X-Bridge Technologies Co., LTD
XIA LLC
XOS

Complete exhibit details including contact information and a description of the products and services can still be

viewed on the exhibit page of the Denver X-ray Conference web site: www.dxcicdd.com.

SPONSORSHIPS

The Denver X-ray Conference Organizing Committee would like to give special thanks to the vendors who sponsored the events at the conference. Chemplex Industries, Inc. very generously hosted the XRF Poster Session; Claisse, Corporation Scientifique, hosted a wonderful celebration during the Plenary session in honor of the 100th Anniversary of X-ray Spectroscopy; and ICDD sponsored the XRD poster session. The poster sessions and the Plenary session were enhanced by the food and libations offered by our gracious hosts and we thank them for their continued generosity and support of the DXC.

MOBILE DXC

Attendees could also use a mobile App to enhance their conference experience by planning their day with a personalized schedule, browse the exhibitors, view maps, and learn about all of the latest announcements and updates. This is the second year that the mobile App was used and because of its popularity, it will be offered again in 2014. Special thanks to Premier Lab Supply for sponsoring the App and enabling the attendees to view conference information with great convenience.

DXC 2014 – A BIG YEAR FOR X-RAYS AT BIG SKY, MONTANA

Save the date for 2014! The 63rd Annual DXC will be held from 28 July – 1 August 2014 at Big Sky Resort, Big Sky, Montana, USA. This is the first time that the conference will be held in Big Sky, and we are looking forward to showing our attendees a new and beautiful area of the country.

There are links on the DXC website to help you familiarize yourself with the area and see the many attractions and activities that Big Sky has to offer to the attendees and their families. Come for the conference and stay for vacation – trust us, you won't want to leave!

The 2014 Plenary session will be "X-rays on Mars". The Organizing Committee is very thrilled to announce the three distinguished invited speakers who will be present at the session: Dave Bish, Department of Geological Sciences, Indiana University; John L. (Iain) Campbell, Department of Physics, University of Guelph; and Samuel M. Clegg, Chemistry Division, Physical Chemistry & Applied Spectroscopy Group, Los Alamos National Laboratory. Do not miss these talks!

CONNECT WITH US!

Stay connected with the DXC and the ICDD by following us on Twitter, Facebook, Google+, and LinkedIn. Visit our website or contact our Conference Coordinator, Denise Flaherty. We are here to help you with any questions or concerns you may have, and hope to see everyone again next year in Big Sky, Montana.

Web: www.dxcicdd.com; E-mail: flaherty@icdd.com; Phone: +1 610-325-9814.

Acknowledgements

ICDD thanks the Denver X-ray Conference Organizing Committee who volunteered their time and expertise all year round to help make the DXC a huge success. We especially would like to thank George Havrilla who has served on the committee for nearly 20 years as a leader for the XRF program and X-ray community. George has announced that he will be stepping down as an Organizing Committee member, and we wish him lots of luck with his new endeavors. We will miss you, George!