

Accuracy in Powder Diffraction IV Program

April 22-25, 2013

NIST
National Institute of
Standards and Technology
U.S. Department of Commerce

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Commission on Powder Diffraction,



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Day 1 22 nd April		
Time	Activity	Chair
08:30 - 09:30	Arrival & Registration. Coffee & Tea	
09:30 - 09:45	Welcome, Laurie Locascio, Director, MML Introduction to program (Madsen, Cline)	James Cline Ian Madsen
09:45 - 10:30	Accuracy in Powder Diffraction – Are we There Yet?	Ian Madsen
10:30 - 11:00	Tea Break	
11:00 - 12:45	Microsymposium 1 – Standards	James Cline
12:45 - 13:30	Lunch Break	
13:30 - 15:00	Microsymposium 2 – Instrumentation	Pamela Whitfield
15:00 - 15:30	Tea Break	
15:30 - 17:15	Microsymposium 2 – Instrumentation (cont'd)	Pamela Whitfield
17:15	Poster session Hors d'oeuvre & Cash Bar (Wine & Beer)	

Day 2 23 rd April		
Time	Activity	Chair
09:00 - 10:45	Microsymposium 3 – Data Collection and Analysis	Arnt Kern
10:45 - 11:05	Tea Break	
11:05 - 13:05	Microsymposium 4 – Structure Determination and Refinement from Powder Data	Jim Kaduk
13:05 - 13:45	Lunch Break	
13:45 - 15:30	Microsymposium 5 – In situ Studies	Robert Dinnebier
17:00 - 19:30	Reception – Smithsonian Natural History Museum	

Day 3 24 th April		
Time	Activity	Chair
09:00 - 10:45	Microsymposium 6 – Quantitative Phase Analysis	Ian Madsen
10:45 - 11:15	Tea Break	
11:15 - 12:45	Microsymposium 7 – Proteins & Pharmaceuticals	Robert von Dreele
12:45 - 13:45	Lunch Break	
13:45 - 15:30	Microsymposium 8 – Mineralogical Applications	Johan deVilliers
15:30 - 16:00	Tea Break	
16:00 - 17:15	Manufacturer's Session	Ian Madsen

Day 4 25 th April		
Time	Activity	Organiser/Chair
09:00 - 10:45	Microsymposium 9 – Pair Distribution Studies and Total Pattern Analysis	Simon Billinge
10:45 - 11:05	Tea Break	
11:05 - 12:50	Microsymposium 10 – Stress / Strain	Andreas Leineweber
12:50 - 13:30	Lunch Break	
13:30 - 14:30	Microsymposium 10 – Stress / Strain (cont'd)	Andreas Leineweber
14:30 - 14:45	Short Tea Break	
14:45 - 16:15	Microsymposium 11 – Where to from here?	James Cline Ian Madsen
16:15 - 16:30	Closing Remarks	
16:30	APD IV ends	

Start	End	Activity	Chair	Speaker
08:30	09:30	Arrival & Registration. Coffee & Tea		
09:30	09:45	Welcome – Introduction to the Program	James Cline / Ian Madsen	James Cline / Ian Madsen
09:45	10:30	Plenary I – Accuracy in Powder Diffraction: Are we There Yet?	Ian Madsen	Robert von Dreele Argonne National Laboratory, USA
10:30	11:00	Tea Break		
		Microsymposium 1 – Standards I	James Cline	
11:00	11:45	1.1 Development and Certification of NIST Standard Reference Materials for Powder Diffraction		James Cline NIST, USA
11:45	12:15	1.2 SI Traceable Diffraction Measurements on the NIST Parallel Beam Diffractometer		Marcus H. Mendenhall Vanderbilt University, USA
12:15	12:45	1.3 The Powder Diffraction File: Recent Developments In Quality Control		Soorya N Kabekkodu International Centre for Diffraction Data, USA
12:45	13:30	Lunch Break		
		Microsymposium 2 – Instrumentation	Pamela Whitfield	
13:30	14:15	2.1 Developments in Synchrotron Instrumentation		Andy Fitch European Synchrotron Radiation Facility, France
14:15	15:00	2.2 Neutron Powder Diffraction with Long Pulses at the European Spallation Source (ESS)		Dmitri Argyriou European Spallation Source, Sweden
15:00	15:30	Tea Break		
		Microsymposium 2 – Instrumentation (cont'd)	Pamela Whitfield	
15:30	16:15	2.3 Laboratory Powder Diffraction: The Last 10 Years		Pamela Whitfield National Research Council, Canada
16:15	16:45	2.4 High Performance Hybrid Pixel Detector and its Applications		Yasukazu Nakaye Rigaku Corporation, Japan
16:45	17:15	2.5 Critical Parameters for Instrument Alignment and Performance Verification of XRD Instrumentation		Martijn Fransen PANalytical B.V., The Netherlands
17:15		Poster session Hors d'oeuvre & Cash Bar (Wine & Beer)		

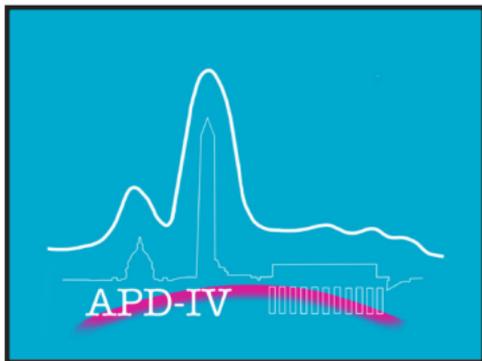
Start	End	Activity	Organiser	Speaker
		Microsymposium 3 – Data Collection and Analysis	Arnt Kern	
09:00	09:45	3.1 Parametric Rietveld Refinement		John Evans Durham University, UK
09:45	10:15	3.2 Developments in Detector Technology for Xray Diffraction		Roger Durst Bruker AXS, USA
10:15	10:45	3.3 Multilayer Optics for X-ray Diffractometry		Bernd Hasse Incoatec GmbH, Germany
10:45	11:05	Tea Break		
		Microsymposium 4 – Structure Determination and Refinement from Powder Data	Jim Kaduk	
11:05	11:50	4.1 Structure Validation in the Submission, Review and Publication Process		Michael Hoyland International Union of Crystallography, UK
11:50	12:15	4.2 Reliable and Highly Accurate Molecular Crystal Structures from a Combination of XRPD and DFT-D		Jacco van de Streek University of Copenhagen, Denmark
12:15	12:40	4.3 Application of Maximum Likelihood Method to Powder Structure Refinement		Takashi Ida Nagoya Institute of Technology, Japan
12:40	13:05	4.4 Crystal Structures from Powder Diffraction: Principles, Difficulties and Progress		Radovan Cerny University of Geneva, Switzerland
13:05	13:45	Lunch Break		
		Microsymposium 5 – In situ Studies	Robert Dinnebier	
13:45	14:30	5.1 Advances in the analysis of in-situ XRPD data using the Method of Maximum Entropy (MEM)		Robert Dinnebier Max Planck Institute, Germany
14:30	15:00	5.2 Non-ambient Diffraction in the Laboratory Environment		Pamela Whitfield National Research Council, Canada
15:00	15:30	5.3 Temperature- and Time-Dependent Cell Parameters During Order-Disorder Phase Transitions		John Evans Durham University, UK
17:30	19:30	Reception – Smithsonian Natural History Museum		

Start	End	Activity	Organiser	Speaker
		Microsymposium 6 – Quantitative Phase Analysis	Ian Madsen	
09:00	09:45	6.1 Current State of Quantitative Phase Analysis		Nicola Scarlett CSIRO Process Science & Engineering, Australia
09:45	10:15	6.2 Accuracy in Quantitative Phase Analysis of Complex Mineral Assemblages: A Decade of Reynolds Cup Round Robins		Mark Raven CSIRO Land & Water, Australia
10:15	10:45	6.3 Rietveld Refinement of Real Structure Parameters of Disordered Clay Minerals in Phase Mixtures		Kristian Ufer Federal Institute for Geosciences and Natural Resources, Germany
10:45	11:15	Tea Break		
		Microsymposium 7 – Proteins & Pharmaceuticals	Bob von Dreele	
11:15	12:00	7.1 Powder Diffraction with Proteins		Jon Wright European Synchrotron Radiation Facility, France
12:00	12:45	7.2 Pharmaceutical Powder Diffraction: Structure Solution From Powder Diffraction Data – How Reliable Are Our Structures?		Maryjane Tremayne University of Birmingham, UK
12:45	13:45	Lunch Break		
		Microsymposium 8 – Mineralogical Applications	Johan deVilliers	
13:45	14:30	8.1 The Impact of Powder X-Ray Diffraction on Mineral Science, Mineral Processing and Process Optimization		Johan deVilliers University of Pretoria, South Africa
14:30	15:00	8.2 Quantitative Rietveld XRD Mineralogy of Copper and Molybdenum Ore Products		Doug Allen Freeport-McMoRan Copper & Gold, USA
15:00	15:30	8.3 Use of Cluster Analysis of XRD Data for Ore Evaluation		Thomas Degen PANalytical B.V., The Netherlands
15:30	16:00	Tea Break		
16:00	17:15	Manufacturer's session – 7 presenters x 8 minutes each	Ian Madsen	

Start	End	Activity	Organiser/Chair	Speaker
		Microsymposium 9 – Pair Distribution Studies and Total Pattern Analysis	Simon Billinge	
09:00	09:45	9.1 Complex Modeling: Towards More Robust Nanostructure Refinements		Simon Billinge Columbia University, USA Brookhaven National Laboratory
09:45	10:15	9.2 Modelling Biomolecules in Solution: Pitfalls and Challenges		Sylvia McLain University of Oxford, UK
10:15	10:45	9.3 Total Scattering Developments for Nanoscale Research		Katherine Page Los Alamos National Laboratory, USA
10:45	11:05	Tea Break		
		Microsymposium 10 – Stress / Strain	Andreas Leineweber	
11:05	11:50	10.1 Microstructure from diffraction: Progress in Line Profile Analysis		Matteo Leoni University of Trento, Italy
11:50	12:20	10.4 Microdiffraction to Analyse Polycrystalline Materials		Henning Friis Poulsen Technical University of Denmark, Denmark
12:20	12:50	10.3 Internal Stresses in HCP Metals		Mark Daymond Queen's University, Canada
12:50	13:30	Lunch Break		
		Microsymposium 10 (cont'd) – Stress / Strain	Andreas Leineweber	
13:30	14:00	10.2 Description and Interpretation of Microstrain (-like) Line Broadening		Andreas Leineweber Max Planck Institute, Germany
14:00	14:30	10.5 Diffraction Analyses of Mineralized Tissue		Stuart R. Stock Northwestern University, USA
14:30	14:45	Short Tea Break		
		Microsymposium 11 – Where to from here?	Cline/Madsen	
14:45	15:30	11.1 Powder Diffraction: The Best Opportunities Are Yet To Come, But ...		Bill David Rutherford Appleton Laboratory, UK
15:30	16:15	11.2 The First X-Ray Diffraction Results From the Mars Science Laboratory		David Bish Indiana University, USA
16:15	16:30	Closing Remarks		James Cline
16:30		APD IV ends		

Accuracy in Powder Diffraction IV

This is the fourth of the “Accuracy in Powder Diffraction” meetings which are held approximately every ten years at NIST. They constitute a review of the state of the art in powder diffraction techniques, instrumentation and data analysis methods. The meeting will host a program of invited presentations plus a contributed poster session. APD-IV will cover the broad range of developments in powder diffraction metrology and methodology in the time since APD-III. In addition, we will host an exhibition area where leading instrument manufacturers and providers will be available to discuss recent commercial developments in the diffraction context.



Logo artwork by Nicola Scarlett, CSIRO Australia

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