

WK4: Frontiers of Materials Research with Single-crystal Total Scattering

Organizers: Stephan Rosenkranz (Materials Science Division, Argonne National Laboratory) and Douglas Robinson (Advanced Photon Source, Argonne National Laboratory)

Location: Bldg. 402, Room E1100/1200

Many physical properties of crystalline materials are strongly enhanced or even driven by local disorder and short-range correlations. These include ionic conduction, thermoelectricity, ferroelectric relaxor behavior, unconventional superconductivity, colossal magnetoresistance, and many more. Their microscopic understanding requires accurate measurements of the total scattering comprising both Bragg peaks from the long-range average order and diffuse scattering from deviations from that average, which includes short-range correlations as well as extended short-range order resulting from defect-defect interactions. Measurements over a large three-dimensional volume of reciprocal space, with sufficient resolution to separate diffuse from Bragg scattering and sufficient dynamic range to include both, are necessary to accurately test models of complex disorder, whether obtained by the use of phenomenological potentials or short-range-order parameters or by *ab initio* methods. New high-energy detectors, such as the recently acquired 2M CdTe Pilatus detector, will also enable the transformation of diffuse scattering into 3D Pair Distribution Functions, which provide model-independent information on the length scales of defect correlations.

This workshop provides a forum for presenting recent developments in instrumentation and analysis that make this technique a powerful tool to investigate complex disorder. It will bring together experts from a wide range of scientific topics to present recent results and the potential impact improved single crystal total scattering instrumentation would have on many fields of great importance to future energy applications.

- 9:00 Stephan Rosenkranz (Materials Science Division, Argonne National Laboratory) & Doug Robinson (Advanced Photon Source, Argonne National Laboratory)
Introduction
- 9:15 Richard Welberry (Research School of Chemistry, Australian National University)
Single-crystal Diffuse Scattering
- 9:45 Thomas Weber (ETH Zurich)
The 3D- Δ PDF Method for Analysing Single Crystal Diffuse Scattering
- 10:15 Break
- 10:45 Branton Campbell (Brigham Young University)
Symmetry-mode Analysis of Local Structure in Complex Solids
- 11:15 Jacob Ruff (Cornell University)
Towards Comprehensive Diffraction Studies of Crystals and Films Using High-

energy X-rays

- 11:40 Ray Osborn (Argonne National Laboratory)
First Results Obtained with the New Pilatus 2M CdTe Detector at APS
- 12:05 Lunch
- 1:30 Marek Pasiak (Institute of Physics of the Czech Academy of Sciences)
Diffuse Scattering in Dielectric Materials: BaTiO₃, PbZrO₃ and Relaxor Ferroelectrics
- 2:00 Bruce Gaulin (McMaster University)
Magnetic and Charge Diffuse Scattering from Geometrically Frustrated Magnets
- 2:30 Alan I. Goldman (Iowa State University and Ames Laboratory)
Short-range Magnetic Correlations in Quasicrystalline i-Tb-Cd
- 3:00 Break
- 3:30 Olivier Delaire (Duke University)
Diffuse Scattering to Study Phonons near Lattice Instabilities and Ordering Transitions
- 4:00 Matt Krogstad (Argonne National Laboratory)
Order-disorder Transition in Na_xV₂O₅
- 4:30 Doug Robinson (Argonne National Laboratory)
Current and Future Capabilities for Diffuse Scattering at 6-ID-D
- 5:00 General Discussion
- 5:30 Adjourn