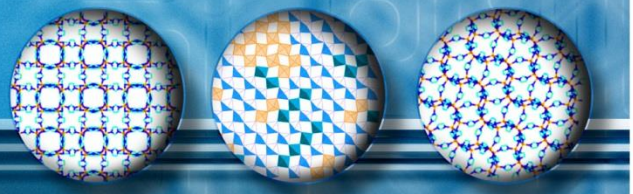
RMCProfile Workshop

February 10–12, 2016

OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE



Functional properties of many technologically important materials are determined by atomic arrangements on the scale ranging from sub-nanometer to several nanometers. Despite availability of experimental techniques that can probe various aspects of local atomic order, elucidating a three-dimensional model that provides a consistent description of atomic arrangements over multiple length scales remains a challenge. The Reverse Monte Carlo (RMC) method has emerged as a promising tool for solving such an inverse problem, enabling simultaneous determination of the local, nanoscale, and macroscopic structures with a single internally consistent model. The RMCProfile computer software enables simultaneous fitting of experimental data from multiple sources, including neutron/X-ray total scattering, neutron Bragg profile, X-ray absorption fine structure, and diffuse-scattering patterns in single-crystal electron/X-ray/neutron diffraction.

This workshop is aimed at introducing neutron total scattering users to the Reverse Monte Carlo refinement method, demonstrating their use in understanding complex functional materials, and reviewing recent developments and future directions in the technique. Half of the workshop will be focused on providing hands-on training with RMCProfile software, with the balance focused on providing a technical foundation and highlighting exemplary work in the community. The final day of the workshop will interface participants with a panel of experts focused on defining challenges and future directions.

Covered topics

- Introduction to RMC Methods
- Modern Total Scattering Instruments and Data
- Hands-on Data Analysis with RMCProfile
- Theoretical and Mathematical Perspectives
- Combining Datasets, Treating Error, and Testing Models
- Magnetic Structures, Frustrated Materials, Framework Structures, Energy Storage Materials, and more
- Participant Contributions

Organizers

Igor Levin, *National Institute of Standards and Technology*
Katharine Page, *Oak Ridge National Laboratory*
Matt Tucker, *Rutherford Appleton Laboratory*

Confirmed Speakers

Martin Dove, *Queen Mary, University of London*
Andrew Goodwin, *Oxford University*
James Neilson, *Colorado State University*
Daniel Shoemaker, *University of Illinois, Urbana Champaign*

For more information visit: http://conference.sns.gov/event/4/

We will accept 30 participants. Preference will be given to active and future SNS users who can benefit from RMCProfile modeling. Selected applicants will be notified on or before December 21. Registration is free. Unfortunately travel support will not be provided.

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