MS27-02 | Recent Developments in the Use of Single Crystal Diffuse Scattering to Study Materials Properties

Rosenkranz, Stephan (Argonne National Laboratory, Lemont, USA); Krogstad, Matthew (Argonne National Laboratory, Lemont, USA); Osborn, Raymond (Argonne National Laboratory, Lemont, USA)

Many physical properties of crystalline materials are strongly enhanced or driven by local disorder and short-range correlations. Examples include ionic conduction, thermoelectricity, relaxor behavior, unconventional superconductivity, and many more. Obtaining a microscopic understanding of such disorder 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. Single-crystal diffuse scattering hence offers a powerful probe of the many unusual physical phenomena that are driven by complex disorder, but its use has been limited by the experimental challenge of collecting data over a sufficiently large volume of reciprocal space and the theoretical challenge of modeling the results. However, recent instrumental advances now allow the efficient measurement over the large three-dimensional volume of reciprocal space, with sufficient resolution to separate diffuse from Bragg scattering and sufficient dynamic range to include both simultaneously, that is 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. Computational advances furthermore enable rapid transformation of large volumes of reciprocal space data into three-dimensional pair-distribution functions that provide model-independent images of nanoscale disorder in real space.

Here, we discuss recent developments of neutron and x-ray diffuse scattering techniques and present results on a variety of phenomena including relaxor ferroelectricity, cation ordering in electrode materials, nematic correlations in iron-based superconductors, and charge density wave correlations.