New Developments in the Use of Single Crystal Diffuse Scattering to Probe Nanoscale Correlations in Crystalline Materials

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Many emerging phenomena of high technological and scientific interest derive from the presence of local disorder and nanoscale correlations embedded within a long-range ordered average crystalline structure. Materials that harbor such disorder often show strongly enhanced responses to external stimuli, with improved properties desirable for future applications. Examples include relaxor behavior, thermoelectricity, ionic conduction, colossal magnetoresistance, unconventional superconductivity, negative thermal expansion, and more. In order to control and further enhance such functional responses requires a detailed microscopic understanding of these short-range ordered correlations. Single crystal diffuse scattering provides detailed insight regarding the existence and morphology of local distortions as well as defect-defect correlations, e.g., the tendency of local disorder to cluster into nanoscale ordered structures [1]. We will discuss recent developments in both instrumentation and novel analysis methods that now provide unprecedented insight into the unusual patterns that persist within short-range ordered states. In particular, the ability to efficiently measure diffuse scattering intensities from single crystals over large volumes of reciprocal space with high dynamic range allows modeling of complex disorder with high fidelity and enables new ways of analyzing the data in real space through three-dimensional pair-distribution functions [2], that can provide model-free images of the nanoscale correlations [3,4]. A novel method to obtain the 3D-dPDF from select regions in momentum space was recently shown to provide novel insight into the origin of structural phase transitions [5]. Finally, recent advances in applying Machine Learning methods to diffuse scattering data can provide new, rapid insight into the information contained in these large data sets [6].

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Work supported by U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division