MS28-02 | Beyond the Average Bragg Structure - Dynamics, Disorder and Diffuse Scattering

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No real crystal shows the periodicity and symmetry implied by its space group. The deviations from this idealized model are static and dynamic. The former encompass atomic positional and substitutional disorder, either in the body or near the surfaces of the mosaic blocks or in both; they cause disorder diffuse scattering below and between the Bragg reflections. Dynamic disorder is due to the omnipresent atomic vibrations and causes the temperature dependent thermal diffuse scattering (TDS). Intensities of diffuse scattering depend on the degree of deviations from symmetry and are generally weaker than Bragg intensities because they are smeared out over the whole of reciprocal space. Multiple atomic positions, occupation factors and atomic displacement parameters derived from Bragg diffraction represent averages over the entire crystals and the time of the diffraction experiment. Diffuse scattering contains information on local structure. Powder diffraction-type, 1D data are interpreted from 1D Pair Distribution Functions (PDFs), single crystal difuse scattering from 3D PDFs which are related to the Patterson function of a disordered crystal. Alternatively, 3D diffuse scattering is modeled with Monte Carlo-type (MC) models of local order. Examples will show how to distinguish static and dynamic disorder from temperature dependent Bragg experiments, how to develop local pictures of occupational disorder from 3D PDFs and how to characterize local structural deformations with MC models. The examples will also delineate the large uncharted territory in the area of crystal dynamics, disorder and diffuse scattering.