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Real-space nanostructure via correlation analysis of scanning microfocus x-ray diffraction data

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Fluctuation scattering techniques (also known as x-ray cross-correlation analysis techniques) aim to extract 3D structural information from scanning diffraction experiments via statistical analysis methods, typically based on correlating diffracted intensities[1]. There are opportunities to study the nanostructure of disordered and polycrystalline materials, nanoparticle assemblies[2] and to image viruses and nanoparticles[3]. These methods use similar microfocus or nanofocus beam conditions to ptychography and spectroscopic mapping techniques and represent a route to add new capabilities to existing spectromicroscopy beamlines. A key challenge for fluctuation scattering methods is interpreting the results in terms of real space structure[1].

Here we present different approaches for interpreting fluctuation scattering results in real-space. As shown in Fig. 1, for disordered samples it is possible to extract the pair-angle distribution (PADF) function which is higher order form of the well-known pair-distribution function[4,5]. We explain how the PADF can reveal 3D nanostructural information in highly disordered materials and show examples from thermotropic and lyotropic liquid crystals[6]. For polycrystalline materials we show how, depending on beam size and domain size, we can gain insights into the microtexture (orientation distribution of the grains) or the structure of the unit cell[7]. We also present an algorithm that can extract crystallographic structure factors to provide a route to structure determination via correlation analysis[8].

There is significant potential to grow these capabilities in a way that is complimentary to existing imaging and mapping techniques, and which may allow access to nanostructural information that is otherwise inaccessible.

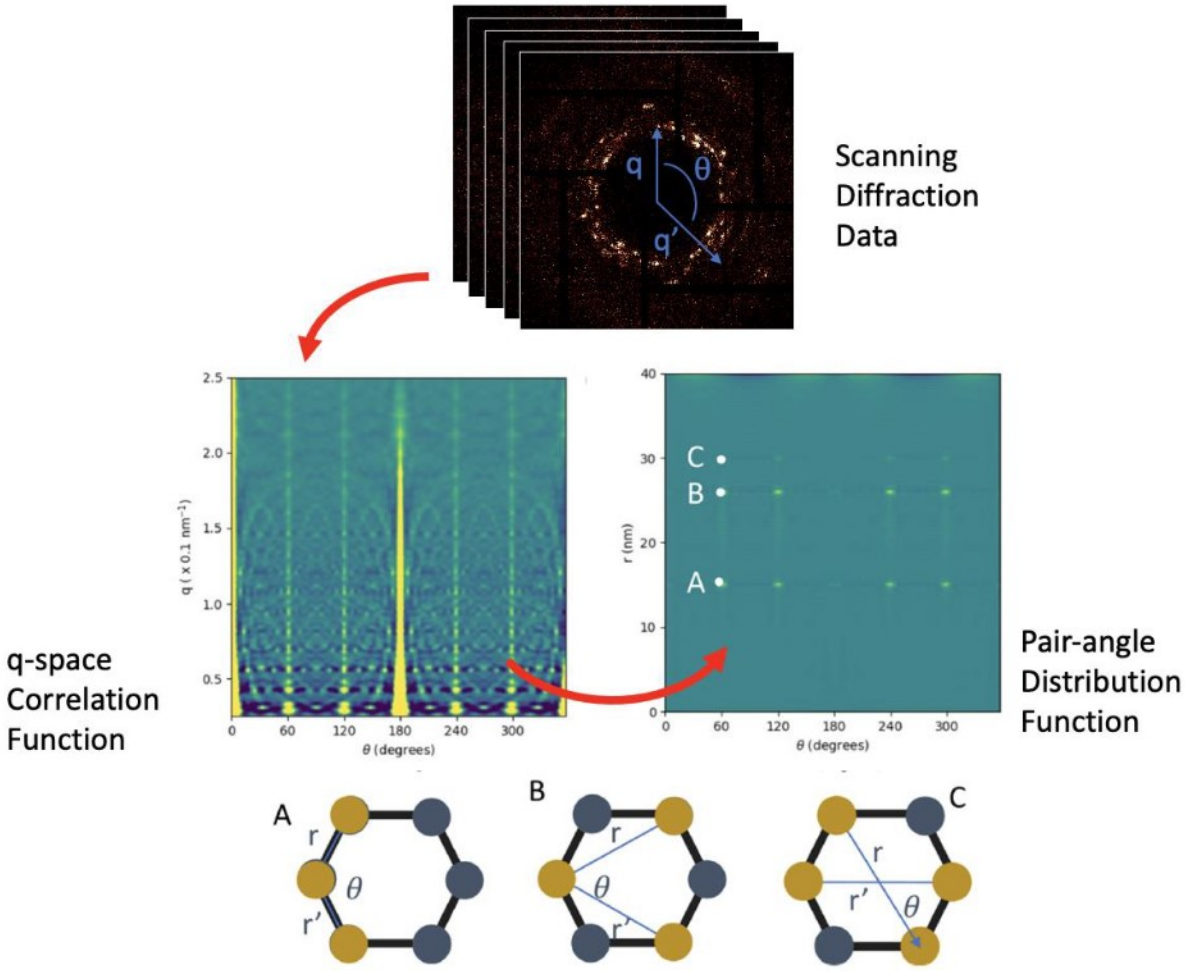

Figure 1. Diffraction data is collected with a scanning focused beam (top). The measurements contain either speckled coherent diffraction or spotty textured rings. These are analysed statistically to produce angular intensity correlation functions (left), which are converted into real-space to obtain the PADF (right). Common combinations of three and four atoms produce peaks in the PADF, allowing the identification of local nanostructure.

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