Coherence in Crystallography for Imaging Materials and Biology

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In crystallography, we consider nanometre-sized crystals to be a new frontier of opportunity to tailor physical properties using 'size' as a control variable. This general view of crystallography "beyond the unit cell" opens a wide field of opportunity for methods development. However, when we think about nanostructures, we must reconsider the standard bulk concepts of lattices and crystal defects. Changes here provide nanomaterials with new and exciting properties. This lecture is about coherence-based methods for the determination of crystal structures using coherence. One example is micron-sized ZnO crystals, attached by bonding to a SiO_2 substrate, which showed internal strain arising from accidental damage during manipulation. Use of more than one Bragg peak from the same crystal allows components of the full strain tensor to be mapped inside the crystal.

These new crystallographic methods have a fundamental need for beam coherence, so benefit directly from 3rd generation synchrotron sources. The coherence leads to interference fringes in the diffraction patterns of sufficiently small crystals. When the fringes are measured using a fine-pixel detector the data can be oversampled beyond their Nyquist/Shannon frequency. To invert the diffraction, we then solve the crystallographic 'phase problem' using a support-constrained HIO algorithm. This leads to quantitative three-dimensional maps of the density of the crystal with a real-space phase, which is interpreted as the deformation of a crystal from its equilibrium lattice spacing.

We have also used the methods to examine twin domain structures within crystals as well as real-space phase domains due to ordering. In biology, we have investigated collagenous tissue, which shows an analogous phase domain structure. For extended objects such as these, we are applying the principles of 'ptychography', in which the crystallographic phase information emerges from overlaps between coherent diffraction patterns.

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