

Coherent Diffraction Imaging of Nanocrystals: Effects of Partial Coherence

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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 talk will illustrate how coherent X-ray diffraction at a 3rd generation synchrotron source can be used to obtain quantitative three-dimensional maps of the deformation of a crystal from its equilibrium lattice spacing. To invert the diffraction, we have solved the crystallographic 'phase problem' by oversampling using a support-constrained HIO algorithm. The ZnO crystals we have been investigating were attached by bonding to a SiO₂ substrate and show internal strain arising from accidental damage during manipulation. Use of more than one Bragg peak from the same crystal has allowed 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. Nevertheless, the coherence is often less than perfect, so we are developing methods to correct for it in the image refinement.

"Coherent Diffraction Imaging of Strains on the Nanoscale", Ian Robinson and Ross Harder, *Nature Materials* 8 291-298 (2009)

"Three-dimensional Mapping of a Deformation Field inside a Nanocrystal", Mark A. Pfeifer, Garth J. Williams, Ivan A. Vartanyants, Ross Harder and Ian K. Robinson, *Nature* 442 63-66 (2006)

"Three-dimensional imaging of strain in a single ZnO nanorod", M. C. Newton, S. J. Leake, R. Harder and I. K. Robinson, *Nature Materials* 9 120-124 (2010)

"X-ray Diffraction Imaging with Partial Coherence", Jesse N. Clark, Ross Harder, Xiaojing Huang and Ian K. Robinson in preparation (2011)