Coherent X-ray Diffraction Images of Nanowires

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Nanomaterials have new and exciting physical and chemical properties. The bulk concepts of lattices and crystal defects must be reconsidered for nanocrystalline matter and structural data are needed. 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 lead crystal we investigated [Nature 442 63-66 (2006)] was grown on a SiO_2 substrate and shows internal strain arising from its external contacts. Closer examination of the strain distribution, after an important correction for X-ray refraction has been included, shows an expansion of the surface layers of the facetted hemispherical nanocrystal. Over most of the surface of the crystal there is a clear outward displacement, which decays exponentially into the bulk. The displacement is suppressed on the (111) facet itself and stronger on the surrounding regions, indicating an orientational variation in surface stress.