Retrieval and Interpretation of Complex Images of Nanocrystals

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Inversion of Coherent X-ray Diffraction is especially interesting when Bragg diffraction from the sample object is considered. First of all, this allows individual objects to be cleanly separated from their neighbours in a typical sample. In this sense it is a "dark field" method. Secondly, the problems associated with eliminating the "direct beam" from the measurements are neatly avoided. However the large momentum transfer involved makes high demands on the quality of the sample: the diffraction becomes highly sensitive to displacements of atoms even at the level of fractions of Angstroms within the object. The nominal "resolution" is much less than this, of course. Being sensitive to tiny displacements can also be an advantage if they can be understood as arising from deformation fields within the sample object.

Here we demonstrate a new formalism that maps the displacement field onto the imaginary part of the object density. In this presentation, we demonstrate the recovery of a 3D image of strain within a lead nanoparticle and show that this is consistent with the theory of elasticity. Phasing the diffraction from the complex object turns out to be no more difficult than for real objects. The method is expected to be general because deformation is common in nanocrystals due to the presence of mechanical strain.