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Electron diffractive imaging of the MgO nanoparticle: Towards atomic-resolution

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Coherent Diffractive Imaging (CDI) involves measuring the oversampled far-field diffraction patterns and reconstruction of the exit surface wave function using iterative algorithms. With the use of electron source it is a promising tool for atomic-scale characterization of individual nanostructures [1]. Practical difficulties of electron CDI include background scattering from the supporting amorphous film, low signal-to-noise ratio, partial spatial coherence of incident illumination and dynamic scattering of electrons. It has also been argued that electron CDI lacks of uniqueness at atomic resolution. For the purpose of exploring computational and experimental applicability of electron diffractive imaging we have performed study of isolated MgO nanoparticles of sizes 10-20nm. The measured intensity distributions around Bragg peaks show continuous diffuse scattering related to the Fourier transform of the shape function. In the data analysis, parameters of the incident beam were obtained assuming partially coherent illumination. For the phase recovery we utilize the difference map algorithm. Sufficiently tight support was dynamically defined by thresholding. Best-fit solution was determined by monitoring the error metric and its uncertainty. Phase recovery procedure, convergence and uniqueness will be discussed in detail.

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Keywords: imaging, phase reconstruction, crystal diffraction

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Coherent X-ray diffraction imaging of non periodic single objects

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Coherent X-ray diffraction imaging (CXDI) is one of the most promising lens-less imaging technique to study the structure and behaviour of non periodic single objects or non periodic assembly of objects at the nanoscale. The first CXDI experiments were performed using planar incident waves (1,2) while the significance of CXDI with curved wavefronts has been demonstrated by Williams et al (3) using a zone plate as primary optics to produce a coherent X-rays point-like source. A successfully Fresnel CXDI experiment with hard x-rays was recently performed using two planar crossed waveguides as optical elements, leading to a virtual point-like source (4). The coherent wavefield obtained with this novel set-up, was used to illuminate a test single object (butterfly). This pioneering work first brought together three concepts - the use of waveguides to produce a coherent X-rays point-like source, X-ray in-line holography, and iterative retrieval of X-ray diffraction phases in Fresnel geometry. A digital two-dimensional in-line holographic reconstruction of the test object was straightforwardly obtained via Fast Fourier Transform of the raw data at a source size limited resolution of 200 nm. A 50 nm diffraction limited spatial reconstruction of the single object was achieved by phase retrieval techniques. Perspectives to nanosized single objects will be discussed.

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3. H. M. Quiney et al. Nature Phys. 2 101 (2006); G. J. Williams, et al., Phys. Rev. Lett. 97, 025506 (2006).
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Beam divergence in electron diffractive imaging

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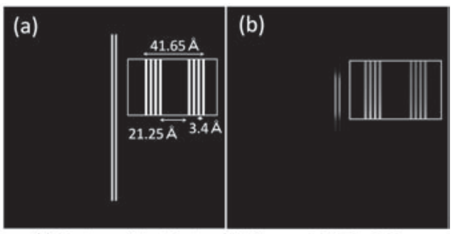
In recent years, diffractive imaging has been developed for material science. Using this method, one can reconstruct the structure of an object from a diffraction pattern [*Nature* **400**, 342 (1999), *Science* **300**, 1419 (2003)]. An image of 3.4Å wall-band spacing of a multi-wall carbon nanotube (MWCNT) has been reconstructed based on a diffraction pattern using a prototype microscope with a 20kV electron beam without a post-specimen lens [*Appl. Phys. Lett.* **92**, 024106 (2008)]. We found that the reconstructed size of an object is limited to the transverse coherence size, which is affected by beam divergence. In the presentation we discuss the influence of beam divergence on diffractive imaging. The beam divergence of a diffraction pattern can be described as a convolution. Due to this convolution, the result of numerical simulation with the parameters used in the experiment shows that the reconstructed object is limited to the smaller size (Fig. (a) and (b)). A new method of deconvolution is proposed for the convoluted diffraction pattern with Poisson noise. Using the proposed method, we recovered the lost area from a retrieved image obtained by the experimental diffraction pattern.



(a) Structure of the object used in the numerical simulations
(b) The influence of beam divergence on diffractive imaging, σ=1.5

Keywords: diffraction imaging of non-crystalline specimens, electron diffraction techniques, deconvolution