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Quantitative Analysis of Crystal Defects: Towards 3-Dimensional Imaging of Charge Densities and Atomic Structure by Inline Electron Holography

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One of the prerequisites for understanding structure-property relationships in advanced materials is the availability of the relevant information. While macroscopic materials properties are often quite obvious, determining the structure of nanomaterials poses a serious challenge, especially, when it comes to point defects and their 3-dimensional (3D) atomic structure. At least equally challenging is the determination of ~~§-dimensional~~ 3D charge distributions, mainly because of the requirement for extremely sensitive techniques for measuring them.

Transmission electron microscopy (TEM) images, in the context of focal series reconstruction (inline holography) over a large defocus range [1], are very sensitive to relative atomic positions and variations in the electrostatic potential and with that charge densities [2]. Although claiming to be able to provide data on the 3D distribution of atoms, this is not true for destructive methods such as the 3D atom probe [3] because the atoms being 'imaged' are not extracted from their original environment but from the sample surface. The enormous advantages of TEM imaging come at the price of the lack of a general direct interpretability at atomic resolution. Although modern electron optics has been able to produce more directly interpretable images by removing many of the additional contrast features owing to coherent lens aberrations, in many cases the images are still not directly interpretable because of the multiple (or dynamical) scattering of electrons within the sample itself.

In this talk, besides introducing a new scheme of atomic resolution tomography which makes use of the fact that electrons scatter multiple times within the specimen (see Fig. 1) for reconstructing its 3D distribution of the electrostatic potential (see Fig. 2 and also Ref. [4]) I will demonstrate how inline electron holography may also be applied to reconstruct variations in the local mean inner potential (see Fig. 3) and the associated 3D distribution of charge densities. I will also show that, compared to off-axis electron holography, inline holography has the potential for being much more sensitive to the presence of charge [5].

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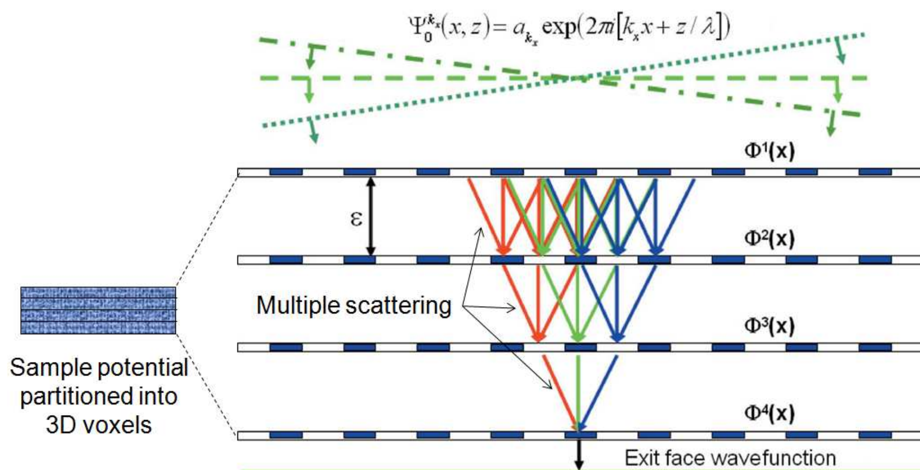

Figure 1: Multislice approximation to dynamical scattering in real space. The scattering of the incident electron beam described by a plane wave is approximated by a finite number of scattering events at equidistant layers partitioning the sample in the z direction. As a consequence, the signal in the exit face wave function is non-local, including contributions from a number of scattering paths, the relative phases of which can be varied by changing the illumination tilt angle $\theta_x = \sin^{-1}(k_x\lambda)$.

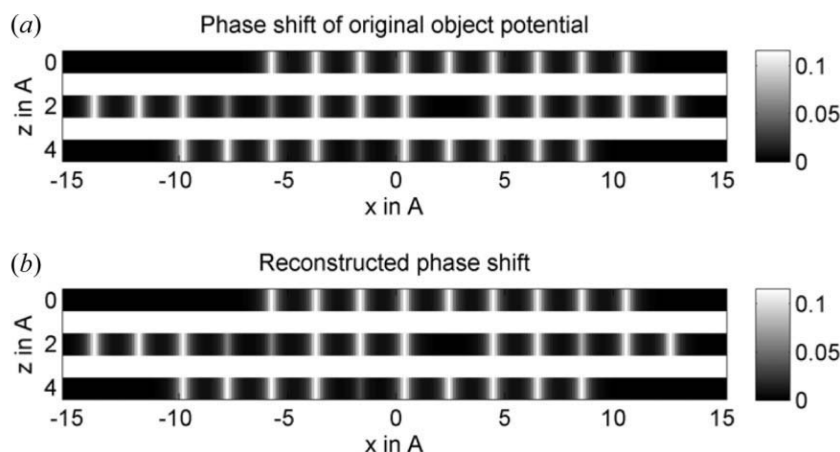

Figure 2: Phase shift $\phi(x,z)=\sigma V(x,z)$ for a three-layered 'phantom' structure (a) and the phase shift reconstructed from it (b), demonstrating a three-dimensional reconstruction at atomic resolution. The accelerating voltage in this simulation was 60 kV, and 5 different tilt angles for the parallel beam illumination between -1° and +1° have been used.

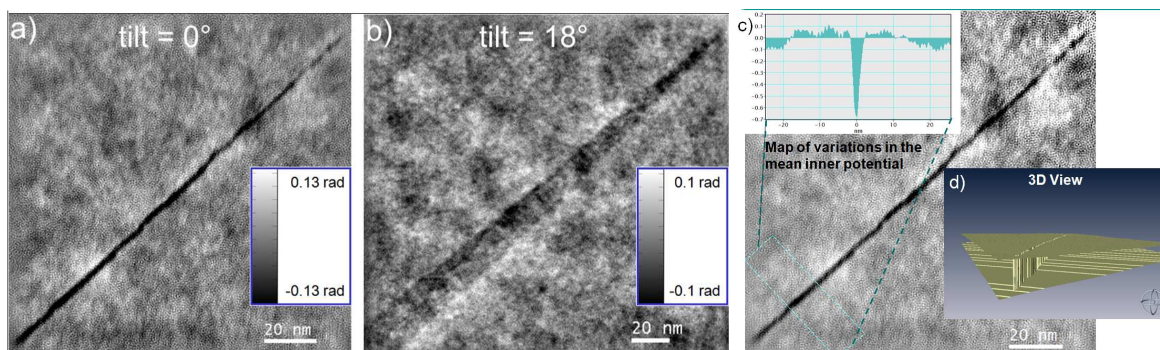

Figure 3: Maps of the relative phase of the electron wave function having passed through a $SrTiO_3$ sample containing a near Σ13 grain boundary at tilt angles 0° (a) and 18° (b). This pseudo-tomographic data set allowed the determination of the precise local specimen thickness and the reconstruction of variations in the local mean inner potential (c) and (d).

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