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Analysis of Phase Difference Variations for Strong Dynamical Objects Using Wigner Distribution Deconvolution Ptychography

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The use of a fast pixelated detectors allow the recording of the full convergent beam electron diffraction pattern for each probe position when performing a scanning transmission electron microscope (STEM) experiment [1]. This results in an information rich 4D-dataset, from which electron ptychography can be carried out [2]. Electron ptychography provides phase images that have been shown to provide structural information of materials at the atomic level [3]. It has been shown that using the Wigner Distribution Deconvolution (WDD) method [4], simultaneous phase imaging of light elements combined with incoherent high angle scattering imaging of heavy elements provides important information of radiation sensitive materials [3]. Moreover, probe aberrations can be estimated from these datasets and accounted for during the reconstruction, leading to aberration-free phase imaging of materials [3]. An assumption on the reconstruction algorithm is that the sample should satisfy the multiplicative object approximation, which usually becomes invalid for strong scattering systems. In this work, we analyze the behavior of the reconstructed phase difference for strong dynamical objects in order to investigate the structural information that electron ptychography can provide from these type of materials.

The study has been carried out on a Pt system in [110] zone axis. Aberration-free frozen phonon multislice simulations using a 200 kV acceleration voltage have been performed using the MULTEM software [5]. The simulations considered a plane wave and a convergent beam with 28 mrad convergence angle for a crystalline structure and for an isolated atomic column 30 atoms thick. Simulations of convergent probe were processed using the Wigner Distribution Deconvolution ptychography method to retrieve the modulus and phase for each thickness. Figure 1 shows the electron wave modulus and Figure 2 the phase difference across the atomic column for a) plane wave simulation of crystal, b) WDD ptychography reconstruction of a crystal, c) WDD ptychography reconstruction of a crystal using aberration correction and d) plane wave simulation of an isolated column for each thickness. These images indicate how the wave propagates inside the sample. Although simulations consider an aberration free probe, we have found that an apparent defocus can be estimated as an aberration as the crystal thickness increases. This has been corrected for and displayed in Figures c).

For the plane wave in a crystal case (a), the broadening and contribution of neighboring columns due to propagation can be observed in combination with channelling effects. In the case of the ptychographic reconstructions (b,c), the channeling effects can be appreciated, but the detailed features related to neighboring column interactions are lost. For the plane wave simulation of a single atomic column (d) only the channelling effects are observable. When comparing b), c) and d), it can be seen that ptychography reconstructions appear to be sensitive to the channeling of the wave but neglect the contributions of neighboring columns. Therefore, ptychography reconstructions appear to be somewhat insensitive to the environment of an atomic column. A discussion on the possible causes for this and how the ptychography method treats this information in the form of probe aberrations will be presented. [6].

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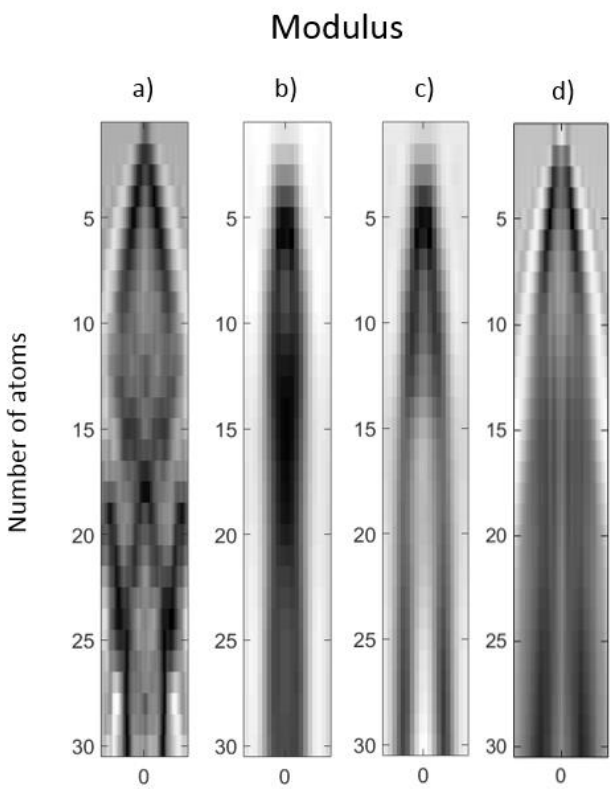

Figure 1. Modulus of electron wave for a) plane wave inside a crystal, b) WDD ptychography reconstruction of a crystal, c) WDD ptychography reconstruction of a crystal using aberration correction and d) plane wave inside an isolated atomic column. Vertical axis corresponds to the number or atoms in the column and horizontal axis is 2 Angstrom distance, in which the atoms are located at the middle (‘0 marker’). Intensity ranges from black = 0 to white = 1

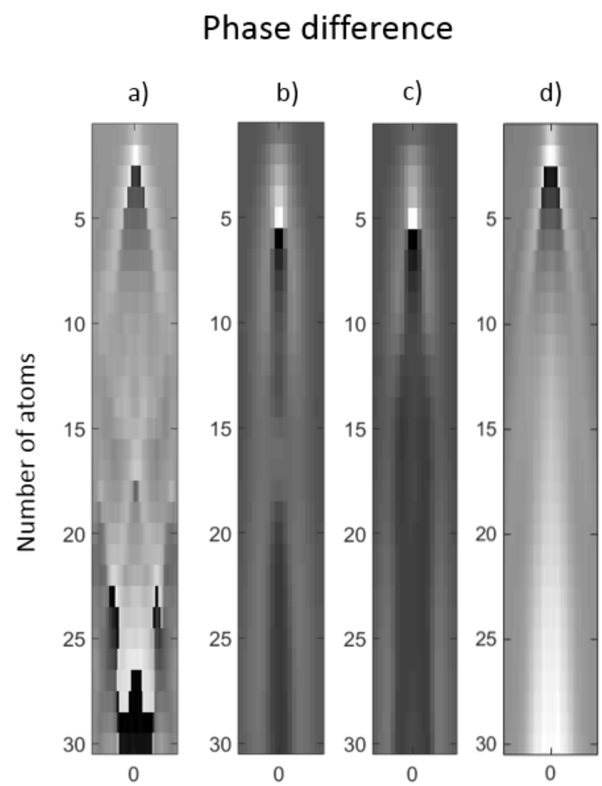

Figure 2. Phase difference of electron wave for a) plane wave inside a crystal, b) WDD ptychography reconstruction of a crystal, c) WDD ptychography reconstruction of a crystal using aberration correction and d) plane wave inside an isolated atomic column. Vertical axis corresponds to the number or atoms in the column and horizontal axis is 2 Angstrom distance, in which the atoms are located at the middle (‘0 marker’). Intensity ranges from black = -π to white = π.

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