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Exploring the Limits of Focused-Probe STEM Ptychography

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The development of high-speed pixelated detectors for the scanning transmission electron microscope is allowing the recording of the 4D STEM data set to become increasingly routine. The data set comprises the two real-space dimensions of the probe scan and the two reciprocal-space dimensions of the diffraction pattern recorded at the STEM detector plane. A powerful and increasingly used application of the 4D data set is the reconstruction of the specimen complex transmission function using electron ptychography. An advantage of the focused-probe mode is that the common incoherent STEM imaging modes, such as annular dark-field (ADF) imaging or energy-dispersive X-ray mapping, can used simultaneously with ptychography for a single STEM scan. It has been shown that the light-element sensitivity shown in the reconstructed phase image can be used in conjunction with the ADF image to enable structural characterization of materials [1].

With electron ptychography becoming increasingly established as a new imaging mode in STEM, it is important to explore the range of potential applications of the technique, and in particular to assess its areas of strength and weakness. Here we explore the phase precision in electron ptychography, and highlight how it can be used to detect the effects of bonding in materials. We go on to use electron ptychography to reveal information about the 3D structure of the specimen, and examine the effects of dynamical electron scattering on the phase reconstruction.

Data was recorded using a JEOL '4D Canvas' pixelated STEM detector which makes use of a pnCCD device [1] fitted to a JEOL ARM200-CF aberration corrected STEM. The detector has a grid of 264x264 pixels and operates at a speed of 1000 frames-per-second (fps). The detector can achieve a speed of up to 20,000 fps through binning/windowing. We typically operate the detector at 2,000 or 4,000 fps, which then dictates the dwell time for the STEM probe.

Figure 1 shows a reconstructed phase image from monolayer hexagonal boron nitride (hBN). For comparison, a simulated reconstruction assuming an independent atom model is presented. It can be seen that the effects of charge transfer due to bonding is readily detected in the ptychographic reconstruction: The independent atom model simulation shows a clear difference in the phase between the B and N sites, whereas they are indistinguishable in the experimental data. For the experimental data, the simultaneously recorded ADF image is required to identify the B and N sublattices. Detailed analysis of the precision of this measurement will be presented.

Figure 2 shows a reconstructed image from a wedge sample of platinum oriented along <110>. Although the phase reconstruction method we use assumes that the sample can be modelled as a multiplicative transmission function, we show that even in thicker samples the reconstructed image shows intensity localised to the atomic columns. As the sample thickness increases, the column intensity does start to become more complex, in particular showing a "donut"-like form. The origins of this form of contrast are discussed.

The appearance of the donut feature can be controlled by manipulating the amount of defocus that is assumed in the reconstruction algorithm. Indeed this approach can also be used to optically section the sample, and we show how effect the method is for 3D imaging of light elements, and also heavier crystalline samples where the effects of dynamical scattering become important [3].

References:

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[3] The authors acknowledge the contribution to the experimental data used below from JEOL Ltd (Y. Kondo and R. Sagawa) and PNDetector (M. Huth, M. Simson and H. Soltau). Financial support from JEOL UK Ltd and the EPSRC (grant number EP/M010708/1) is gratefully acknowledged.

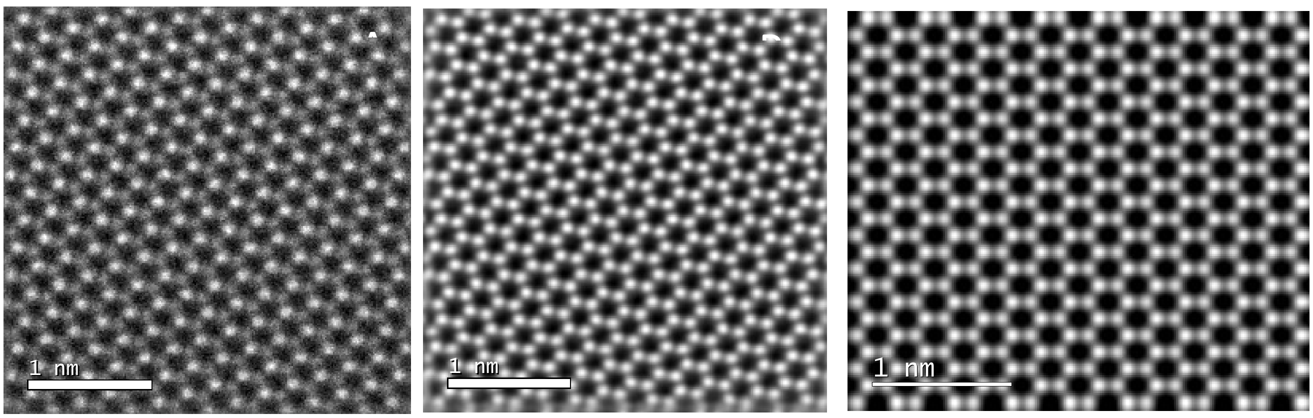

Figure 1. (left) An ADF image of hBN recorded at 80 kV. (centre) The ptychographically reconstructed phase image. (right) A simulation of the ptychographic phase image assuming neutral atoms.

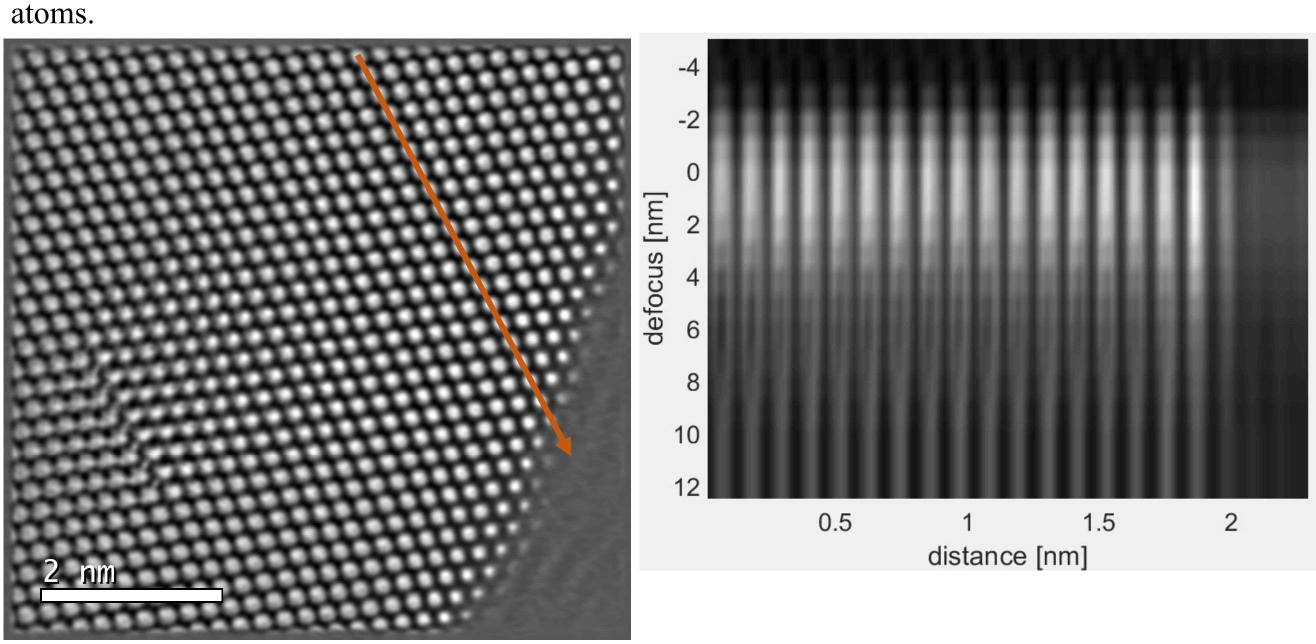

Figure 2. (left) An experimental ptychographic phase image of a wedge sample of Pt recorded at 200 kV. Note the appearance of "donut"-like features in the thicker areas. (right) Phase intensity profiles along the line shown in the image, reconstructed with varying levels of defocus showing how defocus also leads to "donut" profiles for thicker columns that persist to greater levels of defocus.

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