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Quantitative Imaging of Probability Current Flow in Real and Momentum Space

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A new generation of momentum-resolving detectors offers both new physical information about the sample, and also new opportunities to visualize and understand the propagation of the probe electron beam through the sample. We have developed a new electron microscope pixel array detector (EMPAD), with a 1,000,000:1 dynamic range, single electron sensitivity and sub-millisecond frame time [1]. This has allowed us to record the full, unsaturated, diffraction pattern for an atomic-resolution beam scanned across a sample. From this we reconstruct quantitative bright field, dark field and generalized imaging modes that can be compared directly to theory. The detector also allows us to study beam propagation through the sample by measuring probability current flow, which is calculated from the 1st moment of the diffraction pattern $\langle \vec{p} \rangle$ [2]. Here we focus on the physical meaning of the first and second moment generated images ($\langle \vec{p} \rangle$, $\langle p^2 \rangle$), that also gives quantitative insight to differential phase contrast (DPC) imaging, and the optimal imaging conditions by determining effective cutoff angles – a physical realization of strong vs weak quantum measurements.

As the electron probe propagates down the crystal, channeling focuses the electrons onto the atomic columns. Even when the STEM probe propagates along a single atomic column, an oscillation in intensity is seen, and can be understood as a beating between the eigenstates of the system [3]. When two columns are brought into close proximity, additional beatings and oscillations of beam intensity between columns also occurs [4]. In both cases, the oscillating flow of electron in either direction implies a probability current that must also oscillate. The left panel of Fig 1(a) shows the symmetric oscillations when the probe is placed on column, while the right panel shows the flow of the beam on and off the column, resulting in a first moment signal that changes sign with thickness. DPC using a quadrant detector is often used as a qualitative proxy to the true 1st moment (i.e. center of mass) signal [5]. However, even very small misalignments of the crystal or the detector can frustrate this relationship. Fig 1(b) shows the deviations between the DPC and $\langle \vec{p} \rangle$ signals as a function of crystal tilt and sample thickness. Even if the DPC detector were centered, the thickness discrepancies would persist at similar magnitude.

The discussion of momentum becomes more important when it comes to determining cutoff angles for imaging. We can lose information if the spread of momentum in the diffraction pattern is larger than the collection angle. Conversely, we can extract different aspects of the sample by limiting the collection angles. Fig 2(a) shows experimental EMPAD images of $SrTiO_3$ over a thickness range of 0-120nm. We observe that at small cutoff angles the image is sensitive to both tilt and thickness variations. For comparison we use multislice simulations of $SrTiO_3$ within the frozen phonon approximation to generate Fig 2(b). First moment images in Fig 2(b) together with Fig 1(b) implies that crystal tilt dominates while thickness oscillations reflecting momentum flow are heavily damped by large angle scattering. Second moment images are largely insensitive to tilt, and reflect the scattering potential at larger cutoff angles.

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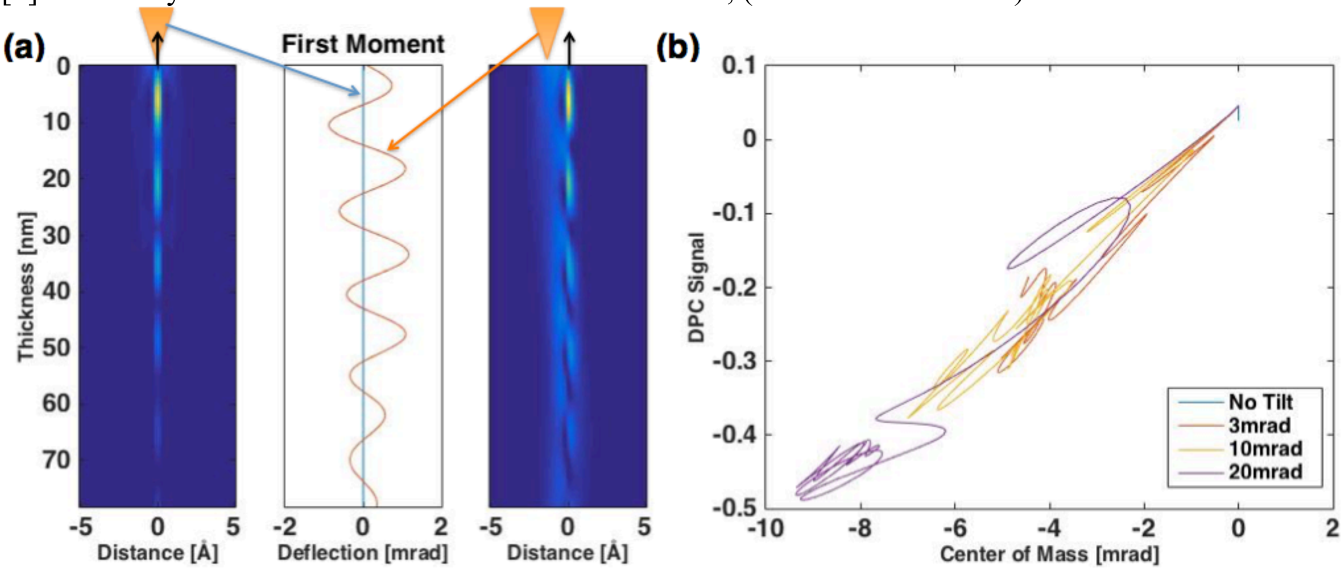

Figure 1. (a) Cross section profile of electron beam intensity versus depth when the probe is exactly on top of an isolated column of Ti atoms and when it is 0.8Å away from the column. The middle plot shows the oscillation of the first moment, which can be understood from the right panel as probability current flow on and off the column. (b) The Non-linear relation between DPC signals and COM for $SrTiO_3$ when the DPC detector is misaligned by one pixel. Large tilts generate larger DPC and COM signals.

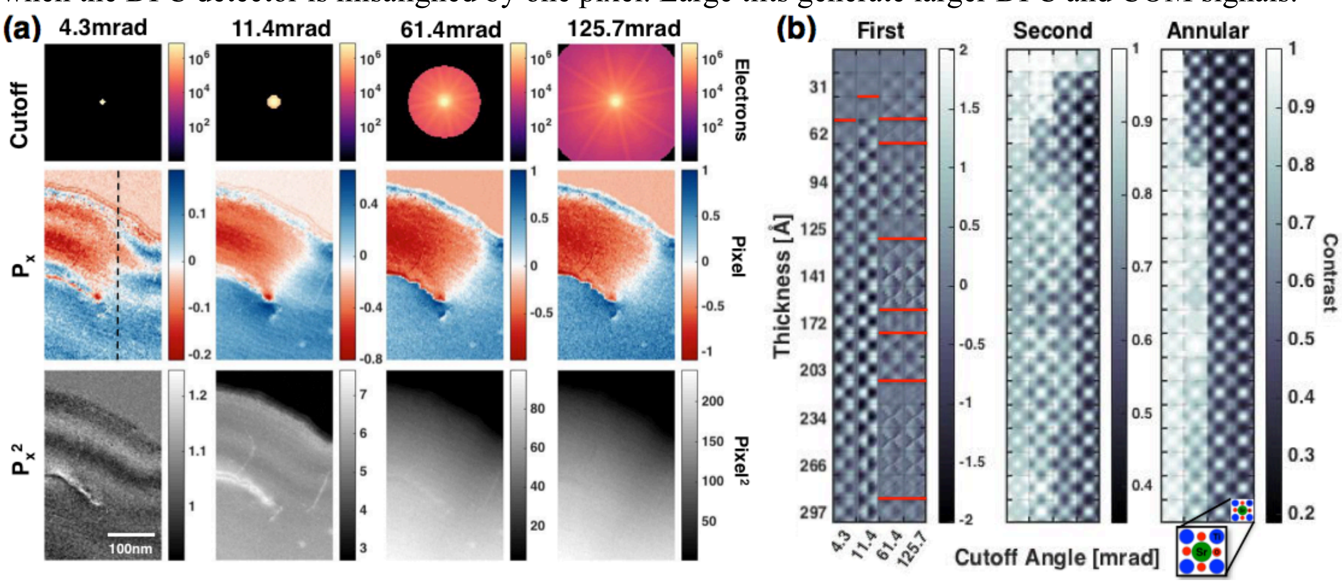

Figure 2. (a) Comparison of experimental $\langle\vec{p}\rangle$ and $\langle p^2\rangle$ images of $SrTiO_3$ with different cutoff angles, processed from 200 keV EMPAD data. In the first moment image at 4.3mrad cutoff, we observe contrast due to tilt on the left of the dotted line. Pure thickness oscillations are seen on the right. (b) $\langle\vec{p}\rangle$, $\langle p^2\rangle$and ADF images of $SrTiO_3$ oriented along the [001] zone axis, at 200keV, 10mrad. Red lines in first moment tableau indicate a sign change. Second moment and ADF images of the tableau are normalized to their maximum value to optimize the contrast in images versus thicknesses.

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