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Comparison of Ptychography vs. Center-of-mass Analysis of Registered 4D-STEM Series

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4D-STEM is gathering momentum, especially for phase measurements, but it is severely limited by artefacts from the serial acquisition process. This abstract has two interconnected parts; the registration of 4D-STEM series as a means to improve the quality of 'raw' 4D-STEM data and a direct comparison of two popular 4D-STEM based atomic resolution phase measurement techniques, namely center-of-mass (COM) based analysis of Ronchigrams [1] and ptychographic reconstruction of sample potential [2-3] using the same data sets.

Despite the enhanced frame rate of modern pixelated detectors, 4D-STEM techniques are severely hampered - especially at atomic resolution - by acquisition speed, which is ultimately limited by the beam current. To enhance the quality of 4D-STEM data sets we demonstrate non-rigid registration of 4D-STEM series that were obtained on our Nion HERMES microscope. To facilitate this, HAADF data recorded together with the 4D-STEM series or even virtual dark field data extracted from the data itself is first rigidly and then non-rigidly registered using SmartAlign [4] and the corrected probe positions are then used to register the whole 5D data set. This is shown in Fig. 1 on the example of a WS_2 monolayer with defects. The data can then be averaged over the series dimension to result in one high quality 4D data set as shown in Fig. 1, or the registered 4D maps can also be individually analyzed as a time series.

Many different approaches exist and are developed for extracting information from such 4D-STEM data sets [5]. Here, we focus on atomic resolution data and present a comparison of projected local charge obtained from COM based analysis of Ronchigrams [1] and potentials derived from ptychography utilizing the same data sets, as shown in Fig. 2. We use our in-house developed ‘Regularized Optimization for Ptychography’ (ROP) code [2] that models the electron propagation through the sample as an artificial neural network and includes a regularization [3]. This code is programmed in C++ utilizing CUDA to harness the power of GPU architecture for the ptychographic reconstructions.

We will discuss how registered and unregistered 4D-STEM data sets compare using the two analysis techniques. This is especially interesting as ROP has a built-in probe position update while the COM analysis assumes the probe positions to be correct to obtain E-field vectors. In addition, the influence of the detector on these two analyses is compared by utilizing data sets from a scintillator-coupled SCMOS camera and from our new Dectris ELA direct detector. Not only do these detectors have vastly different DQE and MTF, but especially the read-out noise is very distinct (zero for the Dectris ELA) and plays a crucial role when low signal is present, as e.g. in the presented case of 2D materials [6].

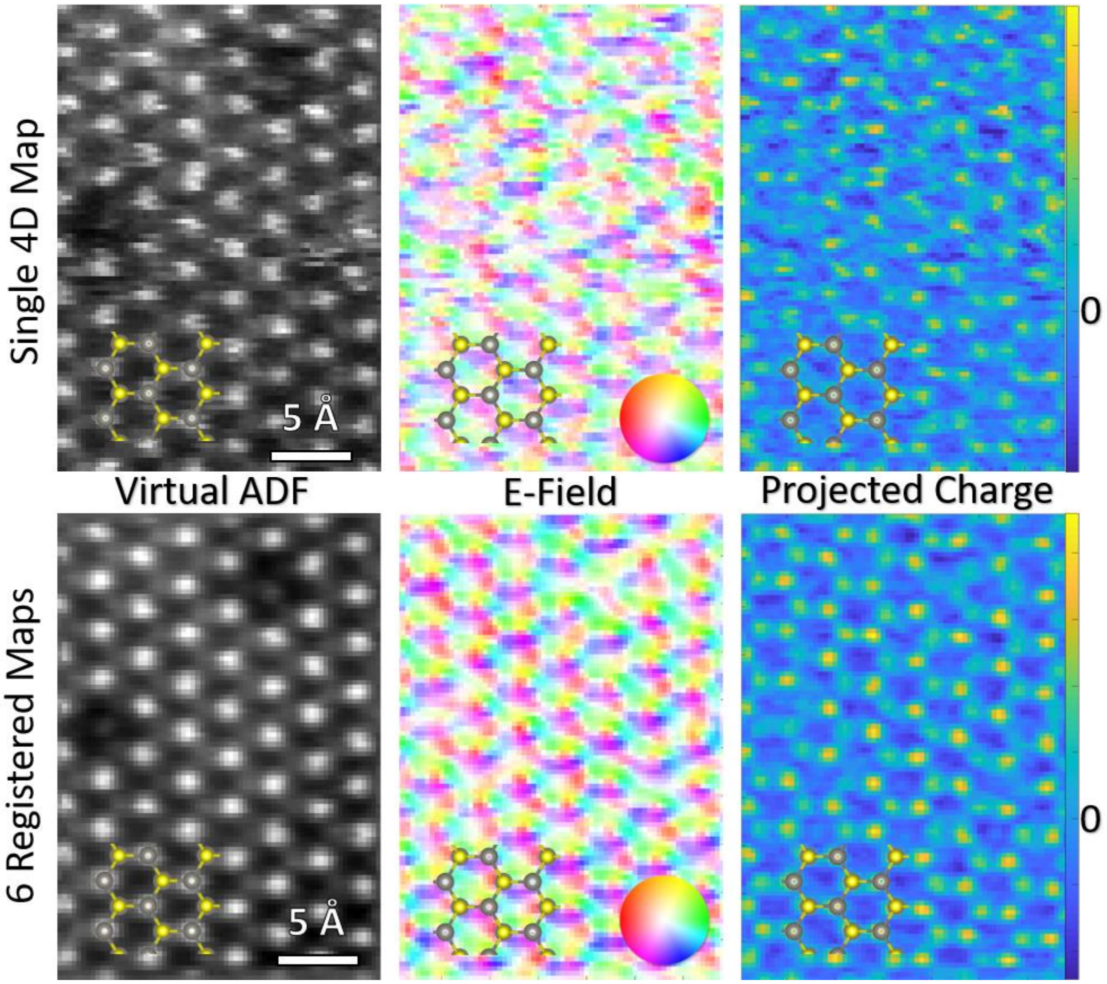

Figure 1. Comparison of virtual dark field, E-field as obtained by center-of-mass analysis of Ronchigrams and projected charge (divergence of E-field) for a single 4D-STEM map (top row) and the average of 6 non-rigidly registered 4D-STEM maps (bottom row) of a WS_2 monolayer with 2 defects. The data was acquired using our Nion HERMES microscope at 60kV and a scintillator-based camera (Hamamatsu Orca) at 1600 frames per second in 128x128 pixels windowed mode utilizing a probe with 35mrad convergence angle and 28pA current. The used scan area was 96x68 probe positions with a pixel-step of 0.313Å.

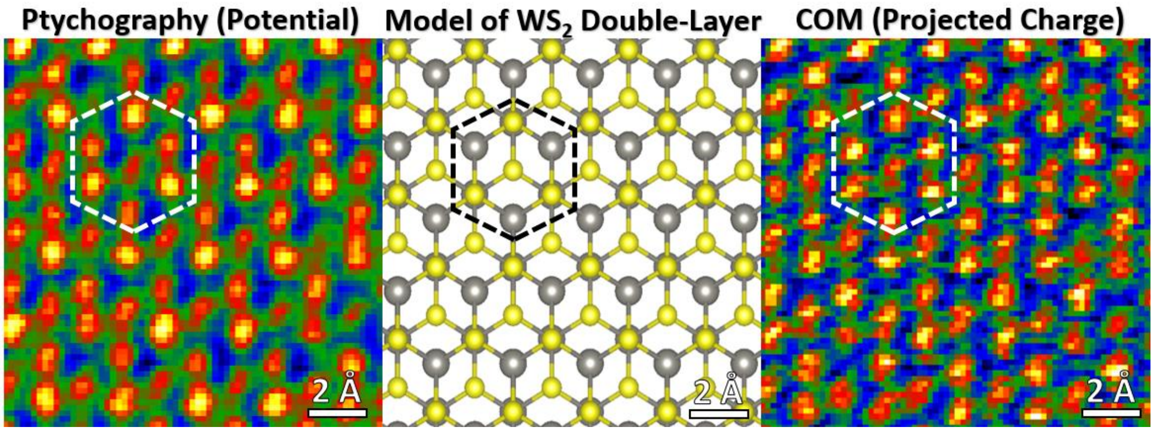

Figure 2. Comparison of phase obtained from ptychography (ROP) and COM-derived projected net charge of a WS_2 double-layer using a single, quite noisy 4D-STEM data set from a scintillator-coupled camera (same parameters as in Fig. 1 but 0.234 Å step size, 40mrad convergence angle and 66x66 probe positions shown). The ptychography-derived data allows to identify the atomic column type while COM does not.

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