Towards Quantitative analysis of electrostatic potential of monolayer WSe2 using electron ptychography

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4D-STEM has thrived thanks to the emergence of fast pixelated detectors in the last few years. The latter enables recording the rich information of the diffraction patterns in STEM [1]. This also makes it possible to map magnetic and electric properties at microscopic scales using methods like Center-of-Mass (CoM) and electron ptychography. Compared to conventional imaging techniques in STEM, electron ptychography enables imaging of the materials beyond the aberration-limited resolution with an optimal use of electron dose. The resolution achieved by this technique was demonstrated to be as small as 20 pm [2], and the ability to recover the diffraction pattern outside the detector plane allows for super-resolution imaging [3]. Quantitative ptychography, where the potential change over an atom can be directly related to the present chemical species combined with the effect of bonding, will have many applications, but has yet to be demonstrated in literature. Since, to the best of our knowledge, no publication directly compares experimental ptychographic reconstructed phase/potential maps or profiles with simulated data, quantitative ptychography appears still challenging.

In this presentation, 4D-STEM diffraction maps of WSe2 were simulated using abTEM[5]. Then the datasets were reconstructed using electron ptychography on the simulated diffraction maps using different reconstruction algorithms, namely ePIE and difference map (DM), implemented in the PtyPy[4]. The reconstructed diffraction pattern as well as the object function were compared using the ground truth of the input to the simulation, to better understand the strengths and weaknesses of both algorithms. The influence of padding was evaluated on the reconstructed data. Finally, this study allows comparison with reconstructions on experimentally obtained 4D-STEM maps on WSe2 or other 2D materials, intending to develop a method of quantifying the electrostatic potential.

The simulations for the 4D-STEM dataset were done on monolayer WSe2 with focused and defocused probes working at 80 kV with abTEM. The convergence semi-angle is 20 mrad. The diffraction patterns were sampled at 0.41 mrad/pixel and then cropped to a size of 256x256 or 512x512. This results in a collection angle of 51.7 mrad and 103.4 mrad at the edge. The dataset of diffraction patterns of size 256x256 was then fed to the ptychography reconstruction using ePIE and DM in the python package PtyPy: One with added padded zeros around the diffraction pattern up to doubled collecting angle and one without. An extra reconstruction using padded diffraction patterns up to 1024x1024 was done to see if it affected the recovered diffraction pattern. An analysis of a random diffraction pattern generated from the reconstructed probe and the reconstructed object function is shown in Fig. 1. While the reconstructions without padding show a good agreement with the original diffraction pattern, the reconstructions with padding fit the original pattern even better. However, for padded reconstruction, ePIE failed to recover the signals while DM smoothly transits and continues to fit outside the detector region. Further analysis of the power spectrum of the object function exhibits a similar tendency that can be observed: until about 1.65 Å-1, padded ePIE reconstruction (orange dashed profile) matches the input simulation well, while DM matches up to a cutoff at 1.75 Å-1. The same analysis with extra padding up to 1024x1024 shows no significant signal improvement, implying that the effect of padding has a limited reach.

This work presented a possible method to quantitatively analyze the electrostatic potential of the monolayer WSe2. Padding in the reconstruction can improve the resolution, however, is limited. Moreover, the comparison between low-pass-filtered ground truth and reconstructions with a simulated finite-sized detector shows quantitative agreement. Care must therefore be taken in experiments since this finite-size constraint is always present.

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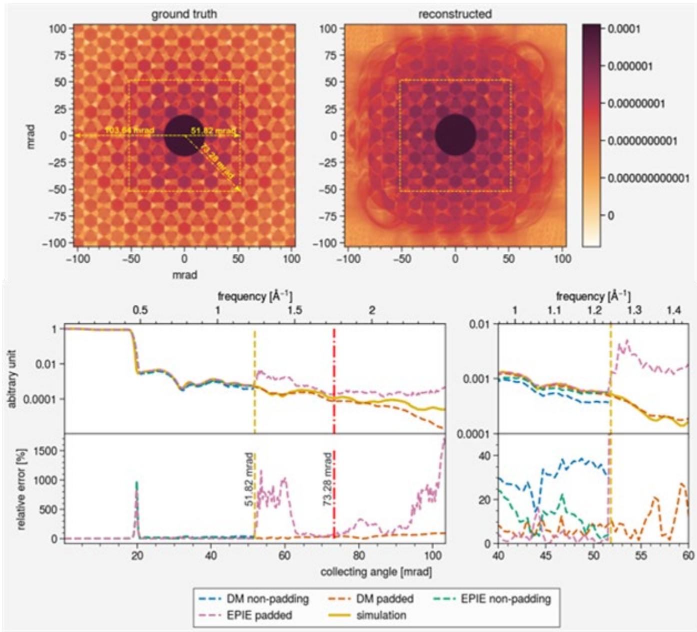
Graphic:



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