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High Resolution Three-Dimensional Reconstructions in Electron Microscopy Through Multifocus Ptychography

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Electron ptychography has rather recently established itself as a technique for high resolution phase-sensitive imaging. Applications have so far focused on radiation insensitive and thin materials. Although ptychography can be combined with the multislice method to generate three dimensional images of thicker samples [1,2], its depth resolution is relatively low and the ptychography reconstruction algorithm can easily face problems of convergence.

The complications inherent to conventional multislice ptychography can be attributed to an insufficient oversampling ratio given the increased number of unknowns that must be recovered in a three dimensional reconstruction. Regularization methods included as part of the reconstruction algorithm have shown improvements of the conditioning of the reconstruction problem and the depth resolution of the reconstruction to some extent [3,4]. A particularly promising one is the missing wedge (MW) regularization that penalizes high axial frequencies k_z at low lateral frequencies k_r of the reconstructed potential V_r in reciprocal space, as shown in Figure 1.

Here, we introduce multifocus ptychography that vastly improves the applicability of multislice ptychography to samples with a thickness of several nanometers. Our implementation uses the gradient based ptychography reconstruction algorithm ROP [3] and uses multiple datasets that have been acquired with a beam focused at different planes. Processing the same type of data, our method can be considered an alternative reconstruction scheme to the recently developed scattering matrix approach for three-dimensional reconstructions from multifocus 4D-STEM data [5].

We demonstrate multifocus ptychography on a lead iridate $Pb_2Ir_2O_7$ (PIO) and yttrium-stabilized zirconia $Y_{0.095}Zr_{0.905}O_2$ (YSZ) heterostructure with a thickness that has been estimated to be 200Å and with a composition of approximately 50Å of PIO and 150Å of YSZ. This sample is the same as used in [5]. Measurements have been performed with an accelerating voltage of 300kV, a 20mrad condenser aperture semi-angle, probe steps of 0.21Å with a dwell time of 0.874ms and beam current of 2.01pA. Four datasets have been acquired with a focus Δf that has been set to 5.3nm, 0nm, -6.2nm and -14.3nm with respect to the specimen surface, respectively. A schematic of the experiment is shown in Figure 2.

The potential was reconstructed in 10 distinct slices separated from each other by 25Å in the z direction. 4 out of the 10 slices are shown in Figure 3. For the multislice ptychography reconstruction, the termination of the PIO layer is evident in Fig. 3a), the transition between PIO and YSZ is indicated by the low phase contrast in Fig. 3b) and Fig. 3c) reveals the uniform crystal structure of YSZ. The reduced quality of the reconstructed YSZ crystal lattice in Fig. 3d), however, suggests difficulties of the reconstruction algorithm to retrieve slices far from the focal plane. An overall improvement of the multislice reconstruction is obtained by using the MW regularization, at the cost of a less obvious transition of the two composites, shown in Fig. 3f). Finally, multifocus ptychography, without applying MW regularization overcomes the issues present in the single dataset multislice ptychography reconstructions. The high reconstruction quality up until the last slice not only reveals the entire structure of each composite in much more detail, the transition between the composites within the heterostructure is now much easier to locate. [6]

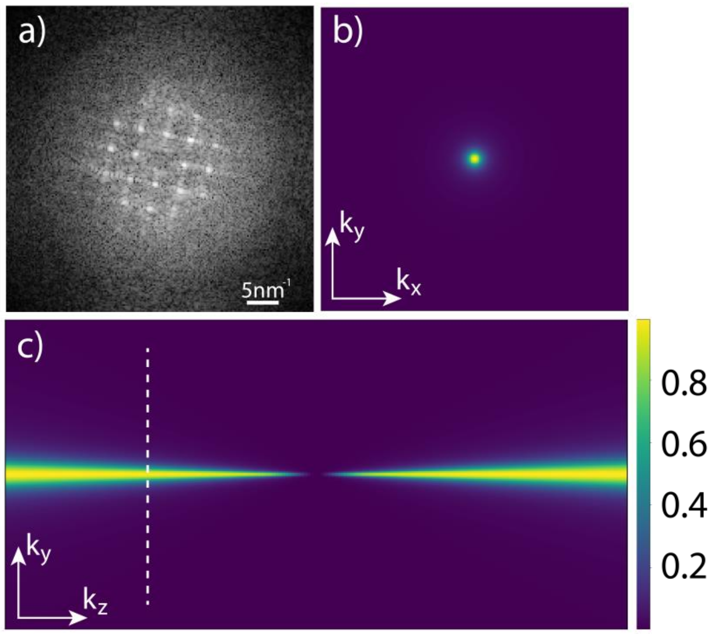

Figure 1. Improved multislice electron ptychography through MW regularization. a) 2D Diffractogram of V_r and b) MW factor applied to the corresponding reconstructed potential V_r in reciprocal space at k_z/k_0 = -0.3, indicated by the white dashed line in c).

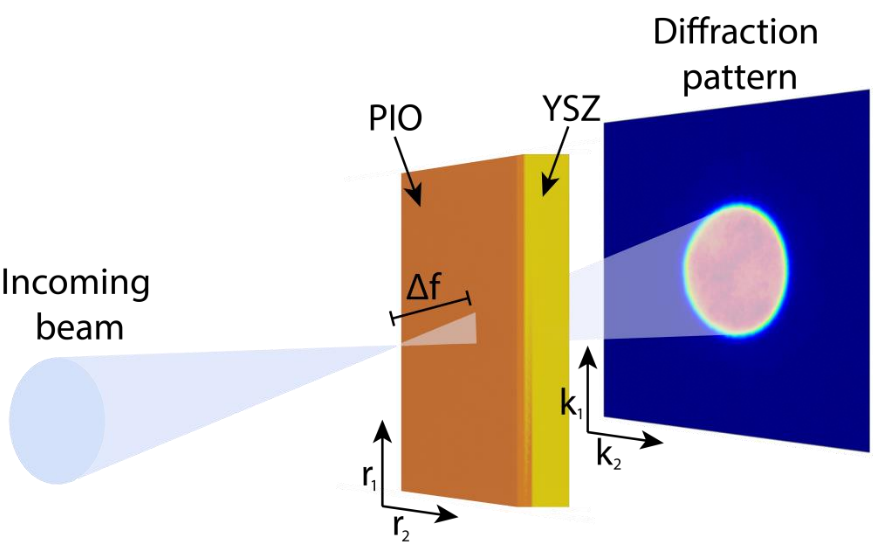

Figure 2. Experimental setup of multifocus ptychography with the PIO-YSZ sample, where each 4D-STEM dataset that is acquired, is defocused by Δf.

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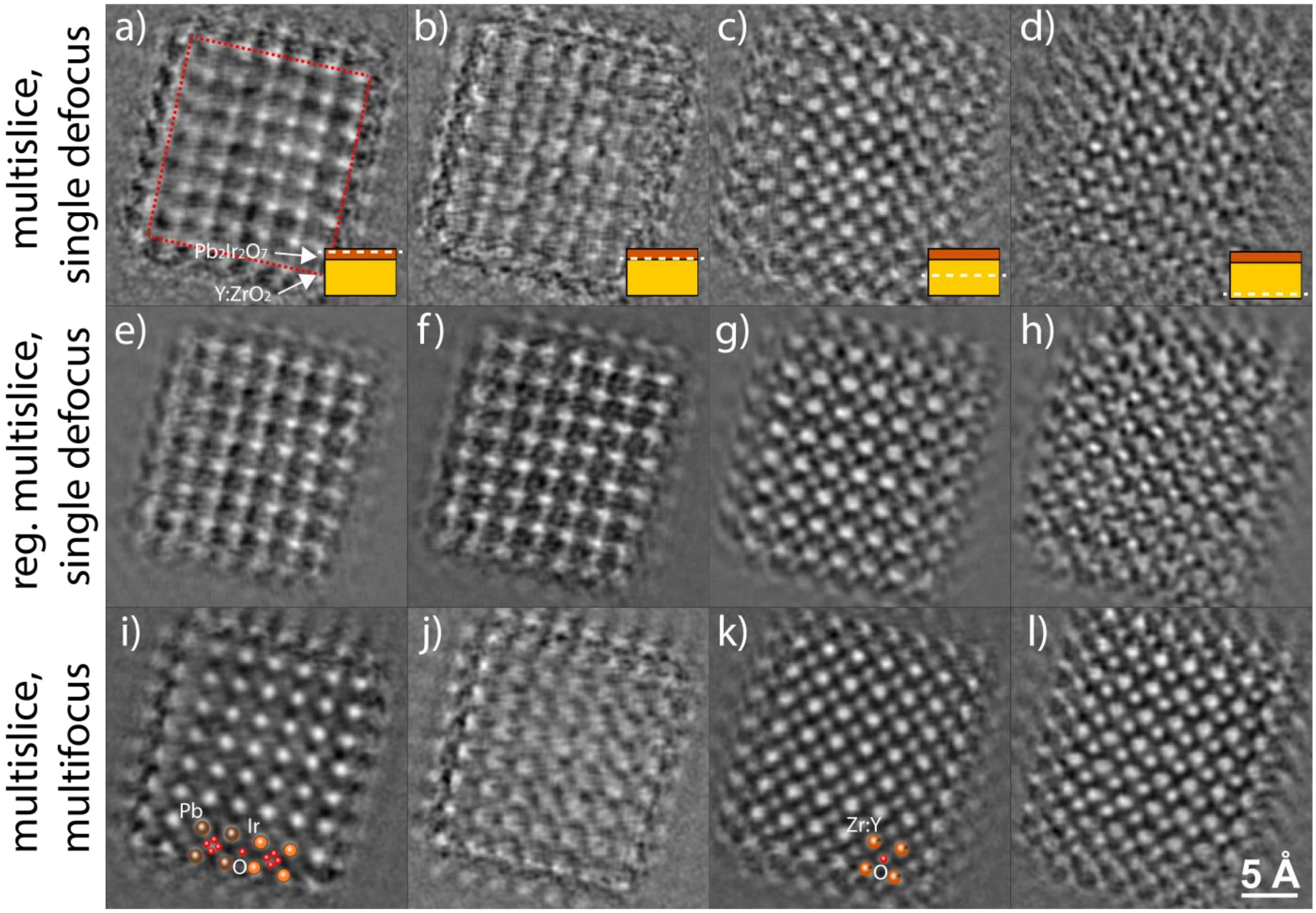

Figure 3. Ptychographic reconstructions of experimental data of the PIO-YSZ heterostructure. a)-d) Reconstructions from multislice ptychography using a single dataset with $\Delta f = 5.3$nm. The scanned area is encircled by a red dashed line in a). e)-h) Reconstructions from multislice ptychography when MW regularization was applied, using the same dataset as in the non-regularized case. i)-l) Reconstructions from multifocus, multislice ptychography using all four datasets and no MW regularization.

References:

[1] W. Van den Broek et al., Physical Review B 87.18 (2013), p. 184108.
[2] A. Maiden et al., JOSA A 29.8 (2012), p. 1606-1614.
[3] M. Schloz et al., Optics Express 28.19 (2020), p. 28306-28323.
[4] Z. Chen et al., Science 372.6544 (2021), p. 826-831.
[5] H.G. Brown et al., arXiv: 2011.07652 (2020).

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