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Meeting-report

3D Sectioning of Rough Interfaces Using Mixed-State Multislice Ptychography, Annular Dark Field, and Integrated Differential Phase Contrast Imaging

Shake Karapetyan[1], Ta-Kun Chen[2], Vincent D.-H. Hou[2], and David A. Muller[1],*

[1]*School of Applied and Engineering Physics, Cornell University, Ithaca, NY, United States*
[2]*Corporate Analytical Laboratories, Taiwan Semiconductor Manufacturing Company, Hsinchu, Taiwan*

*Corresponding author: david.a.muller@cornell.edu

With the introduction of aberration corrected electron microscopes offering a reduced depth of field, depth sectioning of samples became a possibility. However, the depth resolution and fidelity of through-focal imaging using aberration corrected STEM is limited by multiple scattering [1]. We revisit this problem with mixed-state multislice electron ptychography and compare its depth sectioning performance to annular dark field (ADF) and integrated differential phase contrast (iDPC) through focal imaging. To do so, we recover the shape of a known rough interface of a gate dielectric on crystalline Si (a c-Si/a-SiO_2/a-HfO_2 stack) from simulated 4D-STEM datasets. We also report experimental results from the ptychographic reconstruction of a c-Si/a-SiO_2 rough interface. Our results illustrate the robustness of ptychography in real-world experimental conditions for this industrially-relevant interface, overcoming the channeling artifacts present in ADF and iDPC.

Simulated datasets of the c-Si/a-SiO_2/a-HfO_2 rough interface [1] were generated using the abTEM mutlislice python package for STEM at 300 keV with a 30 mrad aperture [2]. As a reference for the expected atomic positions, Gaussian-filtered crystal positions are shown in Fig. 1(a,e); the top panel shows the central slice of the stack, while the bottom panel is the cross section in z along the red dashed line. A single abTEM-simulated dataset was used for a ptychographic reconstruction (Fig. 1(b,f)) using the fold_slice package with mixed-state multislice ptychography [3]. ADF through-focal series (Fig. 1 (c,g)) were obtained from simulations with defocus values ranging from -2 nm to 10 nm, with 1 nm step sizes. iDPC through focal series (with same defocus steps as the ADF series, Fig. 1(d,h)) were obtained by processing the diffraction patterns via an algorithm similar to one used in [4]. Focusing on a single column at the interface (Fig. 1(e-h), marked by the colored arrows), we can see that ptychography provides the most detailed reconstruction. Intensity profiles along these columns (Fig. 2) show that ptychography both provides the highest depth resolution and circumvents the channeling effects in the crystalline portion of the material, as opposed to ADF [1] and iDPC imaging.

As an experimental test, we imaged a c-Si/a-SiO_2 interface from IMEC using a Spectra STEM at 300 kV with an EMPAD detector [5]. Ptychographic reconstruction of the dataset was done using mixed-state multislice ptychography [3]. Fig. 3(a) shows the central slice while Fig. 3(b) shows the depth sectioning along the red dashed line in z direction; interface roughness was observed in both the horizontal and lateral directions. This ptychographic reconstruction of the c-Si/a-SiO_2 interface (Fig. 2(a-b)) shows the sample's wedge-shape, its slight curvature, as well as some information about the roughness in the lateral direction.

Ptychography performed best among the methods used for the 3D sectioning of simulated data and worked in experimental setting as well. Despite the required post processing, ptychography only requires a single dataset for 3D reconstruction of thin specimens, in contrast to the need for multiple images at different defocus values for both ADF and iDPC depth sectioning [6].

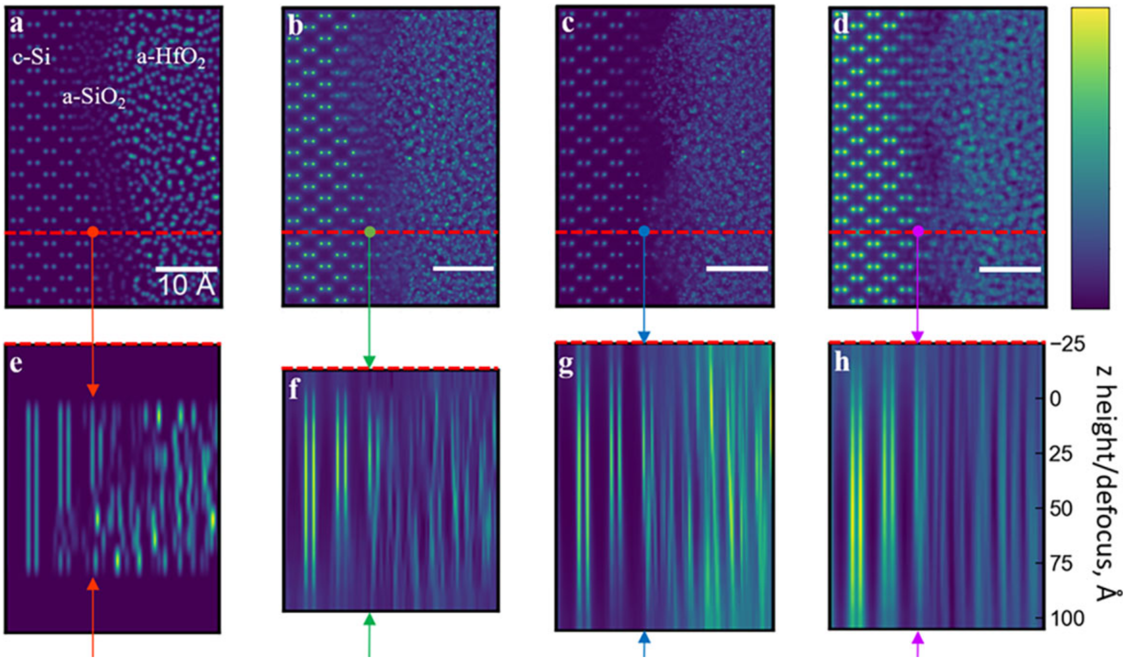

Fig. 1. Simulated images (a-d) and depth sections (e-h) of the c-Si/a-SiO_2/a-HfO_2 rough interface; (a-d) show the central slices of each imaging mode. (a) Reference of atomic positions obtained by 3D Gaussian blurring of atomic sites with 2.5 Å depth resolution. (b) Multislice ptychographic reconstruction of simulated data. (c) Simulated ADF defocus series. (d) Simulated iDPC defocus series. (e-f) Corresponding depth sections of (a-d) along the red dashed line. All scale bars are 10 Å.

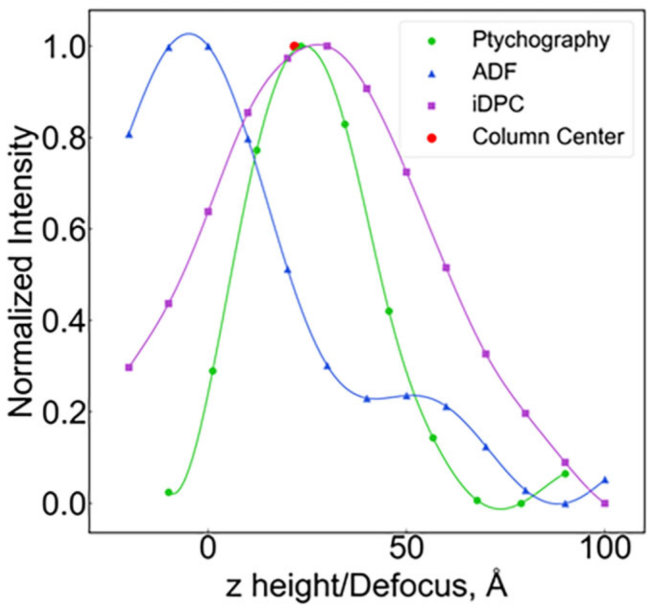

Fig. 2. Intensity profiles along the lines pointed by the colored arrows in Fig. 1. Ptychography (green circles) gives the best resolution and accuracy in z (actual atomic column center marked in red).

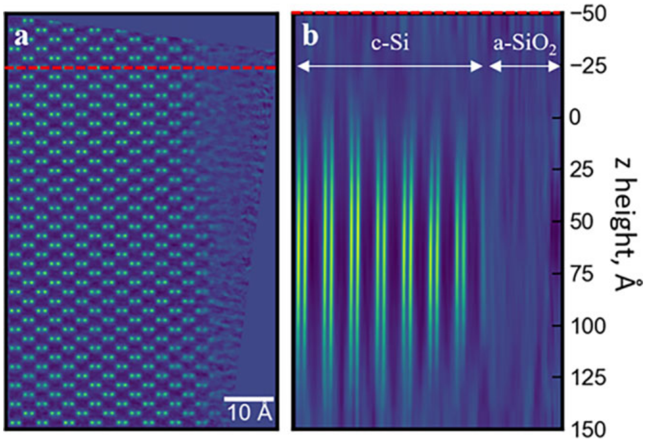

Fig. 3. Ptychography reconstruction of experimental data taken from a c-Si/a-SiO_2 rough interface. (a) Central slice of the reconstruction. (b) Depth section in z along the red dashed line. The reconstruction reveals the wedge shape of the lamella.

References

1. HL Xin *et al.*, *Applied Physics Letters* **92** (2008), p. 013125. doi:10.1063/1.2828990
2. J Madsen and T Susi, *Open Research Europe* **1** (2021), p. 24. doi:10.12688/openreseurope.13015.2
3. Z Chen *et al.*, *Science* **372** (2021), p. 826. doi:10.1126/science.abg2533
4. R Close *et al.*, *Ultramicroscopy* **159** (2015), p. 124. doi:10.1016/j.ultramic.2015.09.002
5. MW Tate *et al.*, *Microscopy and Microanalysis* **22** (2016), p. 237. doi:10.1017/S1431927615015664
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