

Robustness evaluation of electric field measurements via template matching in 4D-STEM

Alexis Wartelle¹, Matthew Bryan², Yiran Lu¹, David Cooper², Jean-Luc Rouvière³, Martien den Hertog¹

¹Institut Néel, CNRS-UGA, Grenoble, France, ²LETI, CEA, Grenoble, France, ³MEM, IRIG, CEA, Grenoble, France

Background incl. aims

Wave-based Scanning Probe Microscopy (SPM) techniques may provide a wealth of information even down to length scales significantly below the probe's extent. Tapping into it is possible thanks to two-dimensional detectors, which enable access to phase and/or absorption contrasts through the beam's interference patterns. The data analysis may then range from complex, stochastic approaches to simple and deterministic ones. One can take phase retrieval in coherent diffraction imaging [1] and center-of-mass (CoM) in field mapping [2-3] via four-dimensional scanning transmission electron microscopy (4D-STEM) as examples. However, with the dataset's enhanced dimensionality (compared to e.g. differential phase contrast imaging with a segmented detector) comes a broader range of field determination methods from which to choose.

Methods

In this presentation, we address the question of reliability in 4D-STEM electric field mapping by way of a comparison between the conventional CoM method on one hand, and several template matching (TM) approaches on the other hand. Our focus being on methodology, we use data acquired on a well-known silicon p-n junction [2-3] for simplicity. The imaged area is a 128-pixels-side square [see Figure 1(a)], with a step size of 5.4 nm, our detector is a 256x256 pixels Merlin camera based on medipix technology from Quantum Detectors, and the TEM is operated at 200 kV. The lamella's large thickness (326 nm of active material) and the electron beam's semi-convergence angle (992 μ rad) allow us to preserve both signal-over-noise ratio and spatial resolution. Most importantly, the small probe size leads to a rigid, lateral shift of the electron beam without intensity redistributions; one may therefore expect good performances from TM.

As a first step, a common reference position (on the detector) for all compared methods is evaluated by averaging the beam's center position over 5120 pixels more than 100 nm away from the junction. We then run a standard CoM analysis along with TM and extract the junction's electric field from the corresponding results, after subtraction of the reference position. It must be noted that the TM algorithm we use (from the liberTEM [4] module) possesses sub-pixel accuracy. Denoting R the estimated beam radius on the detector and r the radial coordinate from the center, the tested, rotation-symmetric templates are: (i) a flat disk with radius R , (ii) the same disk multiplied with r/R , (iii) template (i) with a negative annulus around it, (iv) template (ii) with a negative annulus around it. A final template (v) is created from an actual data frame or the average of several of them.

Results

As can be seen on Figure 1, all templates yield distinct results, and none match the output of CoM. The significant spread in extracted field values suggests high sensitivity to the template's shape, and therefore to user input. That is why we now focus on the template resembling data the most: an acquired detector frame. Since the template (v) was created with a square cropping mask in order to exclude a Kikuchi band from the pattern, we first check whether a disk-shaped cropping mask (with a radius clearly above the beam's) produces different results. Not only is it the case, but we also find out that slightly increasing

the mask's radius strongly affects the template matching output, even though the Kikuchi band was still rejected (only background/weak beam tails were included).

This implies that a correlation-based shift determination places too much weight on absolute intensity levels, failing to accurately locate the pattern's edges. In order to alleviate this, we propose to perform template matching using not a raw detector frame, but the corresponding map (still in detector space) of the norm of its gradient [5]. Our goal consists in evaluating the robustness of this approach versus its two free parameters: the smoothing applied before gradient computation, and the threshold applied on the gradient's norm before TM.

Conclusions

With this study, we hope to improve the understanding of TM's limitations and/or biases in the context of quantitative field mapping. In addition to performing a comparison with CoM, we investigate the performance of two pixelated detectors, using direct detection or CMOS with a scintillator respectively. Finally, we develop an analysis which is guided as much as possible by the data themselves, with the objective to restrict the amount of arbitrariness as much as possible.

Acknowledgements

This project received funding from the European Research Council under the European Union's H2020 Research and Innovation programme via the e-See project (Grant No. 758385). Experiments have been performed at the Nanocharacterisation platform PFNC in Minattec, Grenoble as well as at TEM facility JEOL NEOARM, co-financed by the European Union under the European Regional Development Fund (ERDF, contract n° RA0023813).

Graphic:

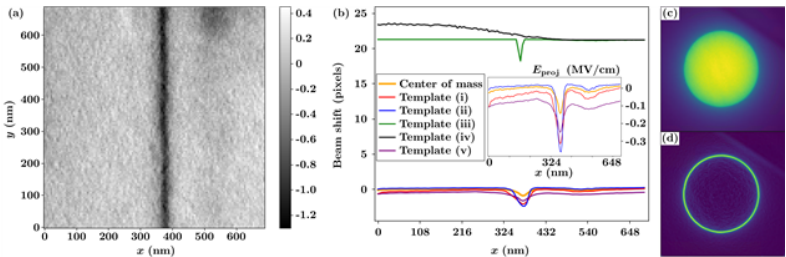


Figure 1: (a) 4D-STEM map of the p-n junction. (b) Extracted average profiles of beam shifts from CoM and template matching; inset: corresponding electric field E_{proj} . (c) Template (v) built from 20 data frames. (d) Norm of the gradient of gaussian-smoothed template (v), $\sigma=1$ pixel.

Keywords:

4D-STEM, CoM, template matching

Reference:

[1] H. N. Chapman et al., J. Opt. Soc. Am. A 2006, 23, 1179-1200.
[2] D. Cooper, L. Bruas, M. Bryan, V. Boureau, Micron 2024, 179, 103594.
[3] B. C. da Silva, Z. S. Momtaz, L. Bruas, J.-L. Rouvière, H. Okuno, D. Cooper, M. I. den-Hertog, Appl. Phys. Lett. 2022, 121, 123503.
[4] A. Clausen, D. Weber, K. Ruzaeva, K. Müller-Caspary, R. E. Dunin-Borkowski, LiberTEM/LiberTEM-blobfinder: 0.5.0. Zenodo 2023.
[5] L. Bruas, V. Boureau, A. P. Conlan, S. Martinie, J.-L. Rouviere, D. Cooper, J. Appl. Phys. 2020, 127, 205703.