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Authors
Pattison, Alexander J
Noack, Marcus
Ercius, Peter

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Automating STEM Aberration Correction via Bayesian Optimization

Alexander J Pattison[1*], Marcus Noack[2] and Peter Ercius[1]

[1.] The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, USA
[2.] Applied Mathematics and Computational Research, Lawrence Berkeley National Laboratory, Berkeley, CA, USA
* Corresponding author: ajpattison@lbl.gov

Multipole aberration correctors have given scanning transmission electron microscopes (STEM) the ability to produce high-quality, atomic-resolution images, enabling STEM to be a key tool in material sciences for characterizing the structure and composition of materials. However, the process of correcting these aberrations typically requires human input and is accomplished using scanned STEM or Ronchigram images at different focii and beam tilts [1]. In these systems, final fine adjustments of aberrations on the sample of interest at the time of data collection are difficult to implement. Furthermore, the need for human intervention and expertise is a barrier to automated experimentation, since aberrations can drift in a matter of hours, reducing the quality of images over time. There exist automated systems for astigmatism and focus optimization, but these typically use exhaustive grid search techniques on crystals and focus on one aberration at a time. With improvements in automation and full computer control, it is possible to reduce the time and dose required to minimize aberrations of any order, ensuring high-quality imaging is maintained throughout a microscopy session.

Here, we demonstrate an automated on-sample aberration correction system using Bayesian Optimization. We have developed a Python-based server able to communicate with the CEOS DCOR aberration corrector and the Thermo Fischer microscope scripting interface. This server allows us to change aberrations, acquire images and perform basic image analysis. In this case, the variance in pixel intensity provides a simple metric for image quality maximization as shown by previous simulations performed by E. Kirkland [2]. The results are fed into a program called gpCAM, which uses Bayesian optimization to update the estimated image quality phase space in search of the best focus (maximum value) [3]. We have tested this system to fine-tune 1st and 2nd order aberrations at high resolution using an atomic lattice and low resolution using separated nanoparticles. The system can simultaneously and efficiently probe multiple aberrations at the same time.

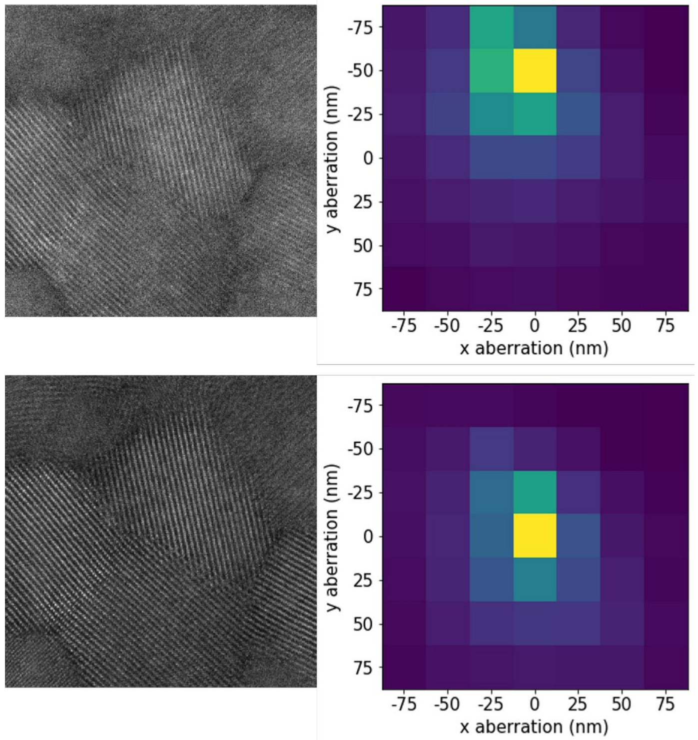

Figure 1. Images and grid searches of pixel variance taken before (top) and after (bottom) automated tuning of three-fold astigmatism (A_2 or $C_{2,3}$) on a poly-crystalline HfO2 thin film.

Figure 1 shows automated tuning of the three-fold astigmatism (A_2 or $C_{2,3}$) on a poly-crystalline HfO2 thin film. The top row shows the aberration state before tuning, with the 7 by 7 grid search on the right indicating an A_2 aberration of 50 nm in the y-direction. We used 50 steps to search for the maximum and Bayesian optimization determined the best image is at A_2 = (-7 nm, 45 nm). A 7 by 7 grid search after corrections shows that the optimal focus was indeed found and the improved image is shown.

Our initial results show that Bayesian Optimization provides a route towards aberration tuning by optimization of ADF-STEM images. Future work will involve simultaneously optimizing multiple aberrations and testing of different image quality metrics on the accuracy of correction. Lastly, we will incorporate this into automated data collection programs to tune microscope alignment without needing human intervention.

[1] OJ Krivanek, et al, in “Handbook of Charged Particle Optics”, 2nd ed., J Orloff, (CRC Press) pp. 601-640.
[2] EJ Kirkland, Ultramicroscopy **186** (2018) pp. 62-65. doi:10.1016/j.ultramic.2017.12.002
[3] M Noack et al., gpCAM v7.3.4, (2022), url:https://github.com/lbl-camera/gpCAM, doi:10.5281/zenodo.5975553
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