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AI Automation for Transmission Electron Microscope Alignment

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Transmission electron microscopes, like other scientific instruments, are becoming increasingly complicated. Consider the I2TEM in Toulouse, a dedicated TEM for electron holography and in-situ research (HF-3300 C from Hitachi) which has a cold-field emission gun, 9 lenses, 4 apertures, 3 biprisms, 18 pivot points to align, and nearly as many elements in the corrector. Operation involves more than one hundred configurable parameters, but with approximately 10^{300} theoretically possible configurations, one wonders if the instrument is used to its full potential. Furthermore, appropriate microscope alignment takes between twenty minutes and an hour each day, depending on the experiment and the microscopist's effectiveness. We propose to explore the use of artificial intelligence to automate the alignment, therefore tackling the complexity and reducing the time taken by the task.

Methods

To address this complexity, we first developed full computer control of the microscope. Hitachi provided access to every single element (including aperture positions, deflector currents and alignment) as well as details about the communication protocol. This enabled us to develop dynamic automation of the microscope to stabilize the specimen and hologram alignment through traditional control and feedback loops in real-time [1]. But to go further, we wondered if the computer could take complete control of the microscope according to the user's needs using artificial intelligence (AI).

Machine Learning, such as Convolutional Neural Networks (CNN), is gradually replacing older forms of automation in various industries. We developed an API to automatically change the microscope parameters while acquiring images (Figure 1). This allowed us to create training datasets for matching the configuration to the images produced by the microscope. Because most configurations would not create an image on the screen, we first aligned the TEM before randomly shifting the parameters around their respective values. This allowed us to predict image characteristics based on the microscope configuration, as well as configurations that met specific image characteristics. In parallel, we have developed a realistic simulation of the I2TEM to produce a dataset of virtual experiments [2] which allows us to test models on various scenarios without the associated cost of directly using the microscope.

Results

This allowed us to train models for each step of the alignment process on the I2TEM (aperture alignment, condenser astigmatism correction, pivot points correction, eucentric position correction and focus correction). The only remaining step is to correct the objective lens astigmatism, which is handled by the corrector using a different API than the rest of the microscope. Each step of the correction, while not as good as human performance yet, takes up to twenty seconds at most, reducing the correction time to less than two minutes. Figure 1 depicts the first step in the alignment: aperture correction.

Conclusion

The results show that AI allows for TEM alignment automation, and while precision is still not on par with human levels, the complex task of finding a good alignment is met, allowing for much faster alignment overall. The method could be extended to other microscopes if they can be controlled via an API and the captured images can be processed in real-time. Additionally, the method used could be modified to address issues like object stabilization, or the calibration of new components.

The aim is to integrate the entire solution into an application that allows microscopists to use the automation functions seamlessly while also allowing them to easily generate or strengthen new automation routines. We are also considering developing a reinforcement learning model that can achieve or maintain a set of meta-parameters according to the user's needs. The meta-parameters are the microscope's parameters that users are most interested in, such as beam size, beam position, focus and magnification, rather than the microscope configuration itself. We intend to encode the image in the meta-parameter space using a constrained variational auto-encoder, with limitations to ensure that they either

coincide with a previously identified parameter, such as the focus, or are at least intelligible to humans. The user can then manipulate the encoded image, and the model will change the configuration accordingly for the microscope to produce an image meeting the user's needs.

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Keywords

TEM, AI, CNN, Automation

Graphic

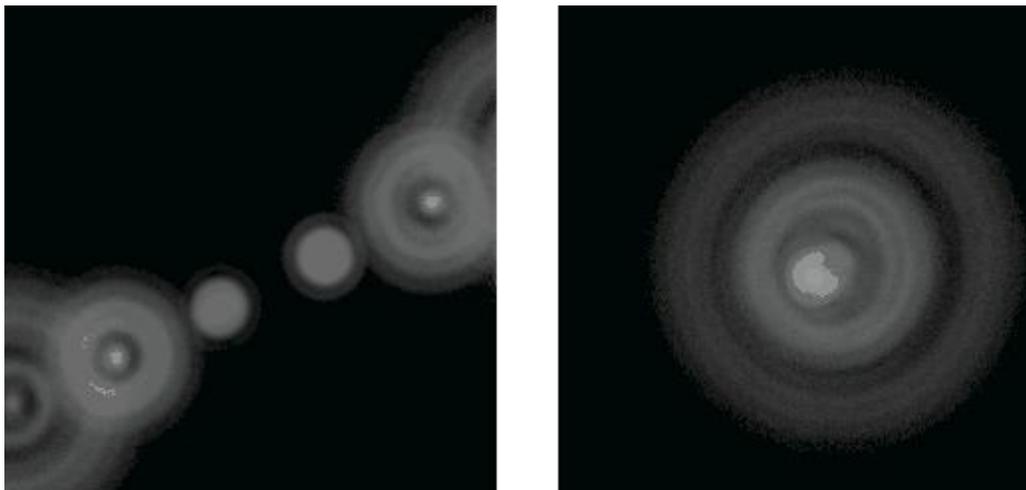


Figure 1 : Example of the i2TEM condenser aperture alignment using the presented ML method (left is before alignment, right after)

Reference:

[1] C. Gatel, J. Dupuy, F. Houdellier, M.J. Hÿtch, Appl. Phys. Lett. 113, 133102 (2018). *Unlimited acquisition time in electron holography by automated feedback control of transmission electron microscope*. [10.1063/1.5050906](https://doi.org/10.1063/1.5050906), [hal-01884057v1](https://hal.archives-ouvertes.fr/hal-01884057v1)

[2] J. Dupuy, Contrôle dynamique et optimisation des observations en microscopie électronique en transmission, PhD Université Paul Sabatier, Université de Toulouse (2021)