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"Push-Button Microscopy": Automated Instrument Alignment and Reciprocal-space Navigation using PyJEM

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This work is a part of Lehigh University's Presidential NanoHuman Interface Initiative (NHI), which aims to integrate the latest advancements in data science, materials engineering, bioengineering, psychology, and human learning strategies in order to disruptively change how human beings harness, visualize, and analyze massive amounts of information. This abstract describes one of many projects the NHI is pursuing to explore potential improvements in human-microscopy interaction and image processing. Specifically for electron microscopy, we have been developing automation processes to control electron microscopes through JEOL PyJEM, a Python-based application programming interface (API) [1] for electron microscopy. In this study, we show several examples of automation procedures that are being developed for a JEOL JEM-ARM200CF aberration-corrected scanning transmission electron microscope (S/TEM). Automation procedures allow users, particularly novices, to focus on higher level activities such as materials characterization and data interpretation, instead of instrument and/or specimen alignment.

The PyJEM package consists of multiple functions to control S/TEM instruments, including stage control (shift in x, y, and z directions and two-axis tilts), optics control (lens strengths and deflections), and image acquisition, both in TEM and STEM modes. We first developed test scripts to confirm the behavior and speed of the PyJEM functions. Then we developed a beam-tilt alignment procedure, known as a coma-free alignment, in TEM mode by combining several PyJEM optics control and image acquisition functions. It is now common practice to apply TEM astigmatism corrections using diffractograms with a recording camera. However, the coma correction, essential for high resolution TEM imaging, requires finding the incident-beam center equaling amounts of tilt-induced astigmation [2]. For this procedure, the incident beam must be tilted and a high-resolution TEM image needs to be acquired sequentially, which is tedious if performed manually. In the PyJEM-based coma-free alignment procedure, the sequential beam-tilting and synchronized TEM image acquisition are automated. As a result, novice users can apply the advanced coma-free alignment more accurately with greater ease.

In addition to coma-free alignment, additional automated procedures are being developed: large-area image montage/stitching with maintaining sufficient image resolution [3] and zone axis orientation adjustments of a crystalline specimen. Image stitching can be used to chart the entire microstructure of a thin specimen and provide a 'spatial navigation' map, in which images taken at a later time can be visually tagged with stage positions using PyJEM. Producing a 'spatial navigation' map is otherwise tedious if done manually. The obstacles of automatic image stitching are the following: (i) collecting a sufficient number of high-resolution images with periodic spacing, (ii) adjusting image brightness/contrast to more seamlessly montage the images, and (iii) automatically adjusting focus in the event that thin specimens are bent.

Regarding development of an automated zone axis orientation procedure, convergent beam electron diffraction (CBED) is used to determine crystal structure and the condition of a thin specimen (e.g. sample thickness or strain) (e.g. [4]). In particular, Kikuchi lines, which are generated as a result of inelastic electron scattering, are used as guides to adjust the sample stage tilts and orient a crystalline specimen to certain zone axes or specific diffraction conditions. Most typically, orienting the thin specimen is performed manually; however, it is challenging for novice users to navigate along Kikuchi lines without appropriate training. Thus, an automated procedure to navigate in the reciprocal space would be useful. The obstacles of the automatic reciprocal-space navigation are the following: (i) there are limited methods to efficiently and accurately extract Kikuchi lines from automatically-collected CBED patterns, (ii) a thin specimen may be bent locally or grains might be too small, both of which can have an unpredictable feature change in the collected CBED pattern after the specimen is adjusted (either via stage tilting or stage translation), and (iii) stage tilt motors are still unable to make precise adjustments to perfectly orient a specimen based on automatic measurements due to the mechanical backrush, inertial motion, etc. Our main accomplishment thus far is the development of an algorithmic, deterministic method for detecting Kikuchi lines from a CBED pattern (Fig. 1).

Overall, this work aims to develop 'push-button' [5] procedures for automating (1) the alignment and tuning of the instrument, including higher-order aberration correction, (2) the construction of 'spatial navigation' maps with automatic image collection, contrast/brightness adjustment and image stitching, and (3) the navigation through reciprocal space to desirable crystallographic orientations, by Kikuchi line detection in CBED patterns and the computation of local grain orientation. PyJEM is used as the main tool to accomplish our goals.

We are now extending our PyJEM-based developments into the latest software platform called JEOL FEMTUS, which offers more integrated, flexible instrument control and data collection in JEOL S/TEM instruments [6].

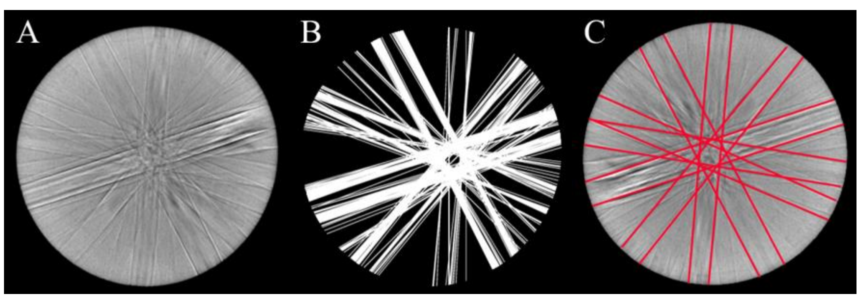

Figure 1: (A) A CBED pattern from Ni, (B) Algorithmically extracted Kikuchi lines, (C) Manually extracted Kikuchi lines (i.e. ground truth).

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