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Meeting-report

Development of an Automated Reciprocal-Space Navigator in a JEOL FEMTUS Platform

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Automating the operations of an electron microscope can benefit many users. Novices, who may be uncertain how to manipulate basic controls, could benefit from automatic procedures that perform specific tasks for them. Expert users could become more productive using procedures that take care of routine activities, such as pre-scanning specimens or aligning the instrument. Regardless of experience level, every user benefits from safety routines that avoid damaging the instrument, and by saving time that would have been spent collecting data.

One common operation, when characterizing crystalline materials in scanning transmission electron microscopy (S/TEM), is navigation in reciprocal space. A thin specimen must be tilted to a certain orientation not only for atomic resolution imaging and analysis but also for characterization of dislocations and various interfaces including grain boundaries. To date, there have been several attempts to develop an automated stage controller for crystalline specimens in S/TEM, including the TEAM stage [1]. However, an automated stage controller for navigating between crystalline orientations is not yet available in a commercial S/TEM instrument. For this reason, we present a system for navigating in reciprocal space using the latest JEOL FEMTUS platform for a JEOL JEM-ARM200CF aberration-corrected S/TEM at Lehigh University.

JEOL FEMTUS has recently been developed for image and spectrometry data acquisition and for various instrument operations including system alignments. In the FEMTUS platform, application programming interface (API) functions for various instrument controls can be accessed via the JEOL PyJEM Python-based library [2]. FEMTUS can thus be used as an integrated development environment (IDE) for python-based scripting. This tool makes it possible to develop automated, flexible instrument control and data collection processes for JEOL S/TEM instruments through the FEMTUS-PyJEM IDE.

To navigate in the reciprocal space, it is essential (1) to identify a current crystallographic orientation of a thin specimen against the incident electron beam direction and (2) to estimate the closest zone axis. Both the steps can be performed by examining Kikuchi lines appearing in convergent beam electron diffraction (CBED) patterns. To automate (1) and (2), Kikuchi lines need to be detected automatically, which we achieved through the following steps in this study.

Prior to Kikuchi line detection, the central part of the diffraction pattern was extracted by applying a mask to remove distorted peripheral parts of CBED patterns (Fig. 1A). Kikuchi lines were extracted by Hough transform-based line detection [3] in polar representation (ρ, θ), which provide a more general mathematical representation for lines in the image than the standard y-intercept and slope in the more recognizable line equation, $y = mx + b$. Here, ρ is the perpendicular distance between the line and the origin, and θ is the orientation of the line. Thus, parallel lines will have the same θ but different ρ values. After line extraction, non-maximum suppression, which merges all detections into the same object, was then performed to select the optimal line. To find a Kikuchi line pair, i.e., a Kikuchi band, θ values obtained through the previous Hough transform-based line detection step were distributed into 72 angular ranges to construct a dictionary of the (ρ, θ) pair. For each (ρ, θ) pair in the dictionary, two adjacent parallel lines with the largest difference in the ρ value were selected to represent a Kikuchi band (Fig. 1B). The crystalline zone axis was estimated by intersections of center lines determined by averaging the ρ values of individual Kikuchi bands (Fig. 1C). It should be noted that the center lines indicate crystallographic planes of corresponding individual Kikuchi bands, and the center-line intersections were calculated by K-mean clustering. Figure 2 compares the zone-axis estimation in three CBED patterns with different zone-axis locations (A: near, B: slightly deviated from, and C far from the optical axis of the instrument). The zone-axes can be estimated almost correctly even if the zone-axis is not located within a center disk of the CBED pattern (Fig. 2C). By calibrating the stage tilt, it is possible to navigate to a zone axis through an automated protocol. The precision of the navigation procedure can be refined further by repeating these steps [4].

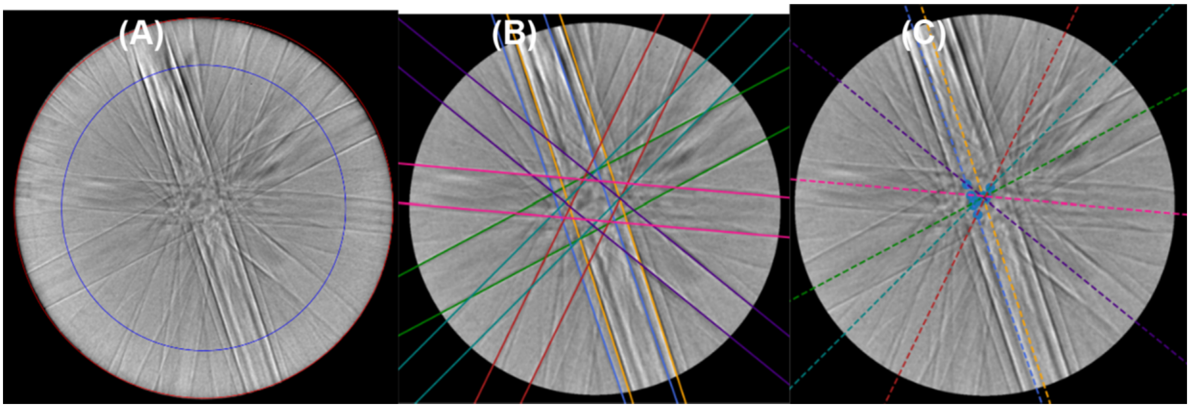

Fig. 1. (A) Application of a mask (a blue line) to select a center area without distortion, (B) extracted Kikuchi lines (colored by pairs) by the line detection, (C) estimation of crystallographic zone-axis through center-line intersections of the Kikuchi bands.

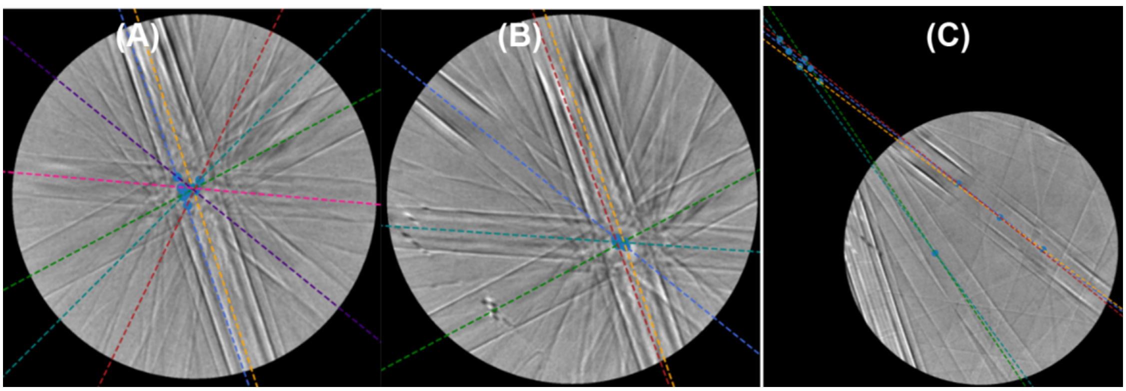

Fig. 2. Results of the zone-axis estimation: (A) near, (B) slightly deviated from and (C) far from the optical axis of the instrument.

References

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