

K-space Navigation for Accurate High-angle Tilting and Control of the TEAM Sample Stage

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The ability to navigate in K-space with confidence, speed and accuracy is an important condition for many experiments in electron microscopy, but despite major advances in stage control, this has remained an elusive goal.

In this talk we present a new software tool that links the coordinates of double-tilt or tilt-rotation stages to crystallographic coordinates of crystalline samples. The tool has been developed as part of the TEAM stage control program, but its use is more general – it can be run in a stand-alone mode and matched to any goniometer by means of linearizing lookup tables and configurable parameters. The software enables sample tilt via a control sphere that can be moved with mouse drags. The control sphere has the same constraints as the actual stage, and can be set to be of tilt-rotation or double tilt type. The stage limits can be configured and displayed on the control sphere, along with the sample's crystallographic coordinates for a simple visual display of all crystal orientations accessible for a given experiment. Sample and crystallographic information is fed into the program in CIF (crystallographic information file) format. CIF files for all crystal systems can be downloaded from numerous databases to save the effort of assembling atomic position coordinate files. Once the CIF loader has extracted all atom and symmetry data, the resulting unit cell can be viewed, and remains synchronized with the stage control sphere. The crystallographic coordinates can be displayed on the control sphere as well, while the corresponding simulated kinematic diffraction and Kikuchi line patterns can be invoked in another window. To align the crystal model with the actual sample, an algorithm has been developed that calibrates the major tilt axis in a few easy steps. Once a sample zone axis and azimuth have been aligned, the tilts for any other crystallographic orientation can be calculated with great accuracy, and the resulting tilt coordinates can directly drive the TEAM stage. Structure factor and diffraction contrast visibility add a quantitative aspect, and this software can also be used for manual diffraction pattern fingerprinting. Figure 1 demonstrates the possibilities of this software with recent results from the newly developed TEAM stage, using an array of Pt-Pd cubes with a size of around 30 nm [1]. This and other examples will be used to illustrate the capabilities of the software and the stage for a number of demanding experiments in electron microscopy.

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Reference:

[1] S.E. Habas, H. Lee, V. Radmilovic, G.A. Somorjai and P. Yang, *Nature Materials* Vol. 6 2007, p. 692 - 696

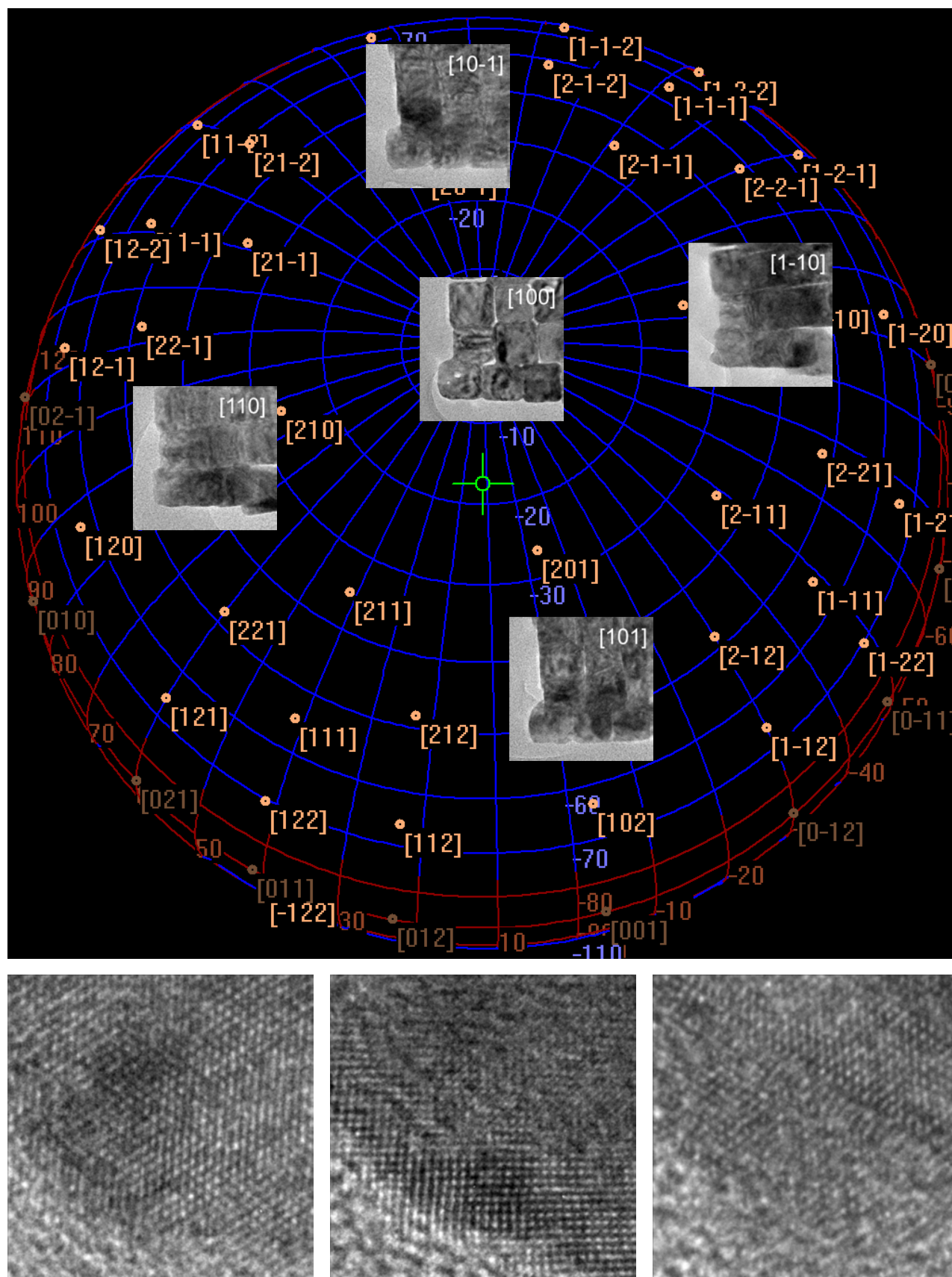


Fig. 1 Top: The graphical output windows of the K-space navigator. Insets show ~ 3 nm cubes in various targeted orientations. Bottom: HRTEM images taken after single-step tilting to [101] (left), [100] (center), [10-1] (right)