Poster

PyFast-ADT: python-driven 3DED data collection and automatic crystal tracking

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3-Dimensional Electron Diffraction (3DED) is a key technique for characterizing nanocrystalline materials, but it is currently limited by not specialized hardware and software [1]. These limitations become relevant when working with *low dimensional* or *highly agglomerated* nanocrystals (few tens of nanometres), as the lack of standard reproducible goniometers with precision in the nanometre scale, require tracking the diffraction volume across a broad range of tilt angles. To address these limits, automating the data acquisition process/algorithm becomes crucial [2]. Here is presented the improved software for 3DED data acquisition PyFast-ADT, a Python-based software designed for data collection of small dimensional materials and *automatic crystal tracking*.

PyFast-ADT is developed for FEI Tecnai SPIRIT and FEI Tecnai F30 Transmission Electron Microscopes (TEM), equipped respectively with a TVIPS XF416R and an ASI Timepix 1 Hybrid Pixel Detector, but *not intrinsically limited* to these setups. The software's flexible architecture allows it to integrate new devices with ease, offering a *standard platform* to continue the developing new 3DED data acquisition algorithms. This is achieved by using *adaptors*, which are abstracted entities containing all the necessary methods for data acquisition, such as illumination mode (TEM or STEM), tilting approach (stepwise or continuous) and camera acquisition method, and specializing them successively for the user defined setup (see Fig 1).

A central new feature of pyFast-ADT is its advanced automatic crystal tracking algorithm, called "Patchwork Cross-Correlation" which replaces previous semi-automatic methods with a *fully automated* approach. This improvement is achieved through an efficient object detection routine that works smoothly with both Continuous Rotation (cRED) and Stepwise Electron Diffraction (PED) methods, resulting in a more reliable crystal tracking path.

As a proof of concept, the *automatic* 3DED data acquisition of two challenging materials is presented. These samples are respectively 15 nm roundish Pseudo Brookite *Nanoparticles* (NPs) and 10 nm (in the short direction) bio-Apatite *needles* from a diseased bones sample, measured both in STEM mode with an electron probe size of *25 nm* (see Fig 2).

Our objective is to provide a solid foundation for new tracking routines and data acquisition strategies in 3DED, leveraging the Python ecosystem to overcome previous hardware limitations, especially for *Scanning-TEM* (STEM) mode. The versatility of Python, with its extensive array of computer vision and image recognition packages, enables the future development of innovative features for 3DED.

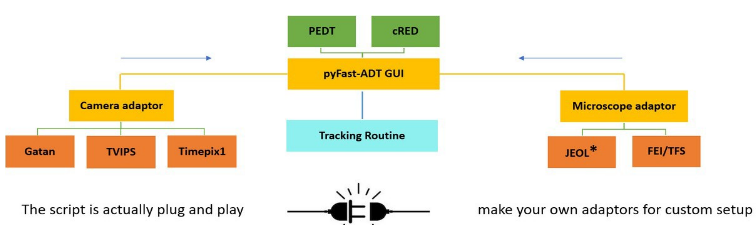

Figure 1. PyFast-ADT software structure. The Graphical User Interface (GUI) is the heart of the software, where the acquisition and tracking methods are implemented. Thank to the Microscope and Camera Adaptor, the software abstracts the behavior of these components, where just a small piece of script specializes the abstracted methods for the specific hardware API used.

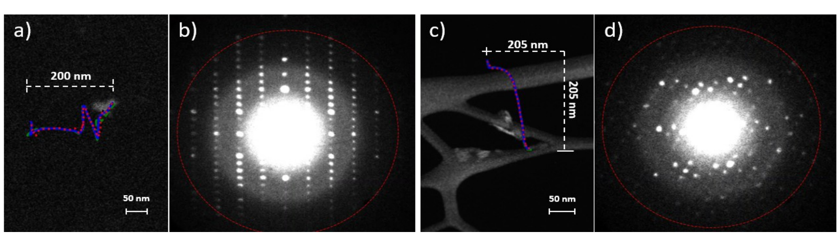

Figure 2. STEM images and diffraction patterns of Pseudo Brookite (a-b) and bio-Apatite crystals (b-d). The result of the automatic tracking paths is superimposed in the STEM images (colored line). The red circle in the diffraction patterns determine a resolution of 0.66 Å.

[1] Gemmi, M.; Mugnaioli, E.; Gorelik, T. E.; Kolb, U.; Palatinus, L.; Boullay, P.; Hovmöller, S.; Abrahams, J. P. 3D Electron Diffraction: The Nanocrystallography Revolution. ACS Central Sci. 2019, 1315– 1329.
[2] Plana-Ruiz, S.; Krysiak, Y.; Portillo, J.; Alig, E.; Estradé, S.; Peiró, F.; Kolb, U. Fast-ADT: A fast and automated electron diffraction tomography setup for structure determination and refinement. Ultramicroscopy 2020, 211, 11295