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Automatic 3D Reconstruction by Deep Learning Neural Networks Using Images Acquired via 4D-STEM Stereo Imaging

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The stereo-pair approach for revealing the 3D distribution of dislocation structures from the transmission electron micrographs proved to be an effective alternative approach compared to laborious electron tomography [1, 2]. Further improvements occurred in the field of stereo 3D reconstruction with the development of a tilt-less imaging technique where a stereo-pair of images can be acquired in a single sample tilt using a convergent probe in scanning TEM mode (STEM) [3]. This technique brings many advantages such as the elimination of sample movement between two images and opens the avenue to dynamic imaging [4]. However, existing algorithms for post-processing and following 3D reconstruction were still slow and required human intervention.

Therefore, we developed a methodology based on tilt-less 3D imaging [3] combined with deep learning convolutional neural networks (CNN) to automatically reconstruct the dislocations network in the 3D volume of a sample. Our approach allows us to automatically detect the dislocation structures and match them on both views without any prior assumptions about their 3D shape [5].

By applying tilt-less 3D imaging [3] on a fast pixelated STEM detector [6] and using our algorithm, we demonstrate the 3D reconstruction of dislocations from virtual stereo-images extracted from the 4D STEM dataset. Fig. 1 depicts the 3D reconstruction procedure from the 4D STEM dataset using a convergence semi-angle of 60 mrad, with a stereo-angle between the images of approximately 6 degrees. Pairs of virtual stereo STEM images can be formed by selecting the two counterpart regions of the direct disc on the diffraction pattern. The images are then treated by CNNs to provide a 3D reconstruction. Our approach delivers the possibility to obtain a larger stereo-angle between the views as well as increases the number of the views on the sample for the following 3D reconstruction and improves its precision. Furthermore, we can optimize the parameters for SNR and angular resolution.

We also extended the tilt-less 3D imaging technique to study the 3D distribution of nanoparticles in cryo condition. We performed the tilt-less 3D cryo-STEM imaging using an annual detector with four segments on the nanoparticles in vitrified ice followed by 3D reconstruction. Fig. 2 depicts our 3D reconstruction pipeline for the nanoparticles. We first perform circle detection on denoised images to detect nanoparticles. When our search algorithm finds consistent detections in all four images for a value of shift on the lines, it is assigned to the particle as its depth. Collecting four images under four different viewing angles of nanoparticles within a frozen solution via single-shot STEM imaging noticeably economizes the time of the experiment and reduces the electron damage of the sample.

Our automatic approach based on deep learning networks allows us to perform fast and reliable 3D reconstruction on various material systems via single-shot imaging using segmented and pixelated STEM detectors. Final 3D reconstruction is represented in the fractional crystallographic coordinates which allow users to extract useful information, for example, dislocation's line direction and habit plane. Our neural networks have been trained with a large dataset from dislocation images in three different materials under various imaging conditions which makes it a versatile tool and a worthy alternative to conventional tomography.

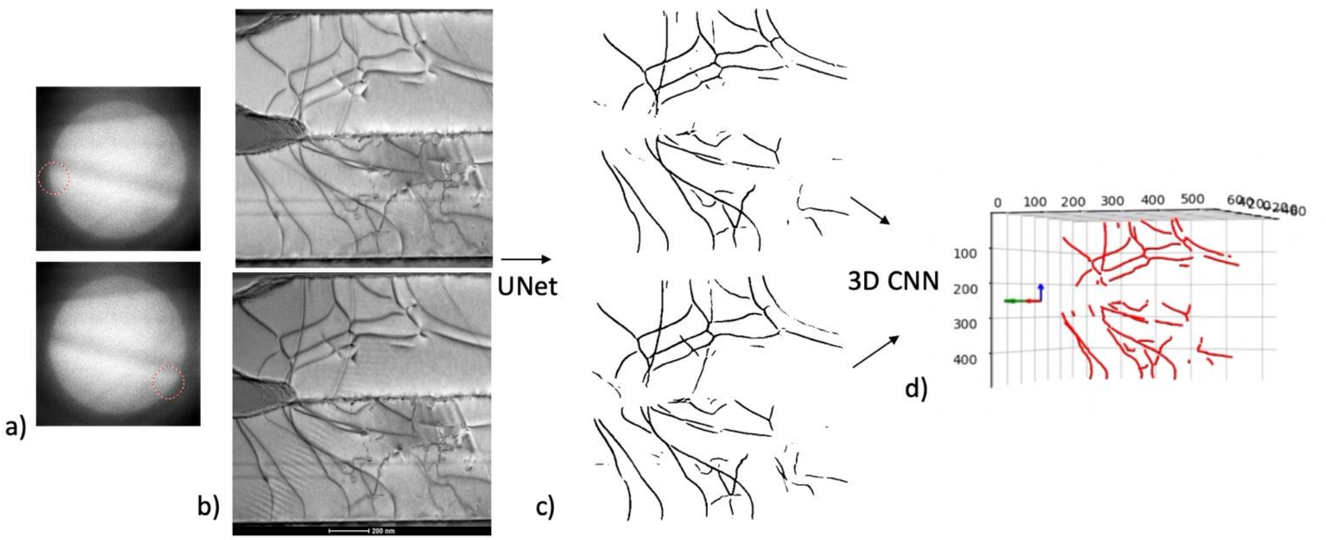

Figure 1. 3D reconstruction procedure from 4D STEM dataset: a) diffraction pattern in 2-beam diffraction condition **g**=(200) acquired on a pixelated detector with projected STEM, b) stereo-pair of virtual STEM images of TiAl alloy from regions highlighted by circles in a), c) corresponding detected dislocations by UNet neural network, d) final 3D reconstruction by 3D CNN.

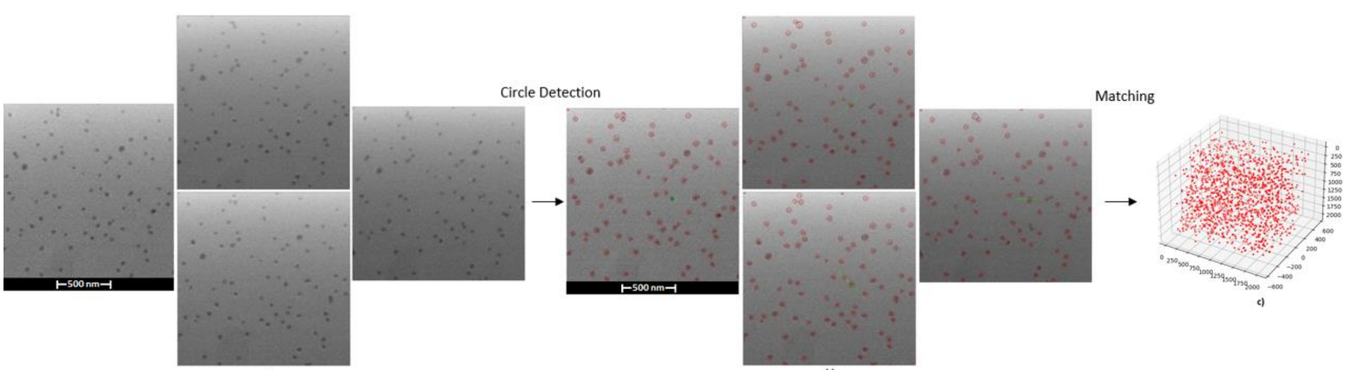

Figure 2. 3D reconstruction of nanoparticles in vitrified ice: a) images from A, B, C, D regions of the detector (shown clock-wise), b) detected particles are shown in red circles. For a chosen particle in region A (depicted as green circle), correspondences are searched on line segments shown as green lines on B, C, D images. c) If consistent detections are found in all 4 images, a suitable depth value is assigned to the particle.

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