STEMcor basic version

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CONTENTS

1 INSTALLATION

You should place the **temDM STEMcor.gtk** plugin into a PlugIns folder of DigitalMicrograph. There are typically several such folders, for instance `C:ProgramData/Gatan/Plugins`.

The script **find plugins folders.s** included in the distribution package will help you to localize desired folders. Open **find plugins folders.s** in DigitalMicrograph and run it by pressing execute or by pressing ENTER with holding the CNTR key. Read the list of available plugins folders. The first folder in the list is most appropriated for placing the temDM plugins.

Some folders can be hidden in Windows. If you do not see all folders, make them visible in the Windows explorer:

Windows 7: Organize tab - Folders and search options - View tab - click show hidden files, folders and drivers checkbox.

Window 10: View tab - click hidden items checkbox.

- Drop **temDM STEMcor.gtk** into the chosen Plugins folder.

- Restart DigitalMicrograph and find the STEMcor in the Menu temDM.

To update the version, just overwrite the plugin of the previous version in the Plugins folder. All versions of **temDM STEMcor** have the same name to avoid confusion with loading ambiguous commands. If you have several versions, it is recommended to keep plugIns in individual folders with meaningful names like `temDM STEMcor basic version 1_XX`.

2 WHY STEM IMAGES NEED TO BE CORRECTED ?

STEM stays for Scanning Transmission Electron Microscopy. Scanning implies moving the probe across the sample in order to form an image. This cannot be proceed very rapidly and typically requires an order of magnitude longer time than shooting fixed-beam TEM images. Since different instabilities (for instance drift of the sample) always exist in the system, a resulted image can be noticeably distorted.

Due to this fact, an operator must always optimize the acquisition time to trade-off between the distortions and the signal counts. Still, it is not exceptional to observe the slightly elliptic shape of the actually spherical particles or to see the monoclinic distortion of the assumable rectangular lattice cell. You are never sure in the proportions of STEM images in fact.

Of course such distortions can be minimized with the instrumental means. Just optimize your tool electronics and wait long enough after insertion of your sample to stabilize it mechanically. However this is sometimes annoying. Whether it is possible to correct for distortions with a software ?
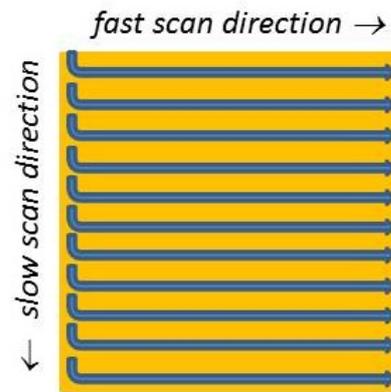
People have suggested a clever way to do that, based on the fact that the STEM distortions depend on the scanning direction. As illustrated in the figure, 2D scanning implies the *fast* and *slow* directions. The distortions within each fast-scanned row are insignificant, while the mismatch among the different rows might be quite severe. Why not scan the same area along different directions and then try to reconstruct an undistorted image ? See, for instance L. Jones et al. Microscopy and Microanalysis 19 (2013) 1050, X. Sang et al. Ultramicroscopy 138 (2014) 28, C. Ophus et al. Ultramicroscopy 162 (2016) 1.

A simplest strategy is taking two images with mutually perpendicular scanning directions. It is apparently very important to keep a minimal pause between two subsequent acquisitions, otherwise the sample drift might shift noticeably your area of examination. Also, the scanning directions must be exactly known for the successful reconstruction. To avoid a mismatch, it is wise to acquire images always in the same way. For instance the **temDM STEMcor** plugin assumes that you first take an *original* image and then an image *rotated* 90° clockwise.

The reconstruction can be executed at the different levels. The basic version of **temDM STEMcor** plugin assumes a linear drift (either mechanical or elec-

tronic) in the course of both acquisitions. Correspondingly, the algorithm estimates such a drift based on the least-square errors method and subtract it from both the *original* and *rotated* images. Most artifacts in the particle shapes and lattice symmetry are gone already after this simplest treatment.

Furthermore, a non-linear drift can be removed with the more sophisticated algorithms. This will be addressed in the advanced version of the **temDM STEMcor** plugin. The non-linear treatment is not a trivial task and typically requires the results of the linear correction as an initial guess. You might try to design your own algorithm and use the output of the basic version of **temDM STEMcor** as your input.
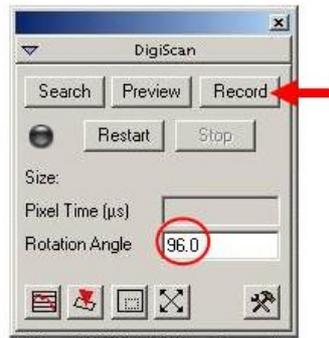
3 HOW TO OBTAIN TWO ROTATED STEM IMAGES

In case you collect STEM images in DigitalMicrograph with the DigiScan tool, then

- start acquisition by clicking Record in the DigiScan palette. You are going to obtain your *original* (unrotated) image.

- after the acquisition of the first image is finished, increment the number in the field Rotation angle by 90. This will rotate your STEM scanning 90° clockwise. To be sure that the new rotation angle is in action press Enter .

- start the second acquisition with the Record button. This will be your *rotated* image. *It is important to keep the minimal pause between two acquisitions*.

- restore the original number in the Rotation angle field
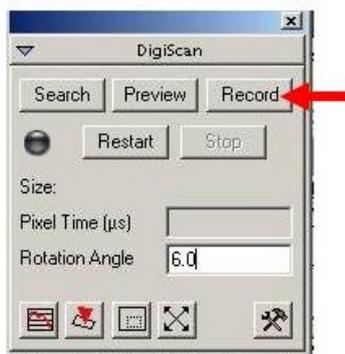
Alternatively, you can use a script for automatic ac-

quisition of two images included in the distribution package. That would save your time and ensure the best results.

- Open **acquire (un)rotated images.s** and check the acquisition parameters - dwell time and the detector index. If you do not know to which index the desired detector is assigned, just try different numbers starting index 0.

- Run the script by pressing execute or by pressing ENTER with holding the CNTR key.

If you employ FEI TIA to collect STEM images, the action sequence is a bit more complicated.
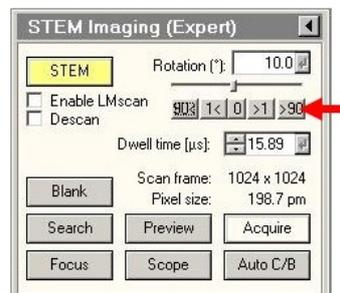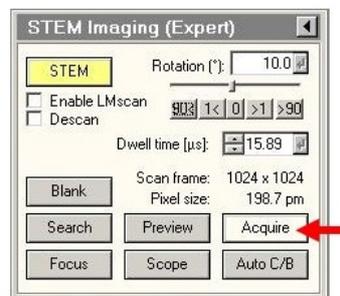
- start acquisition by clicking acquire in the FEI STEM interface.

- when acquisition is finished click the >90 button. That will rotate your STEM scanning 90° clockwise.
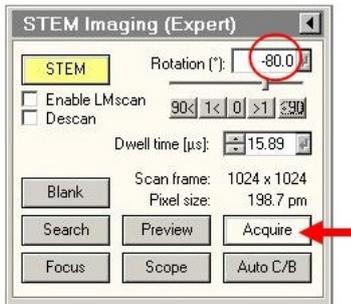
- start the second acquisition with the acquire button. *It is important to keep the minimal pause between two acquisitions*.

- store both images from TIA and immediately close them. Unfortunately TIA does not allow any access to the open files from the other programs.

- Now move to DigitalMicrograph, open the **STEMcor** tool by choosing temDM : STEMcor in the Menu.

- Press the import TIA button and choose the *original* stored TIA file.

- Press the import TIA button again and choose the *rotated* stored TIA file.
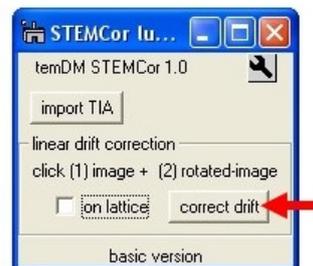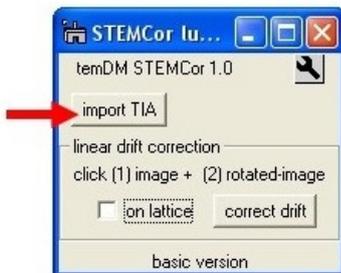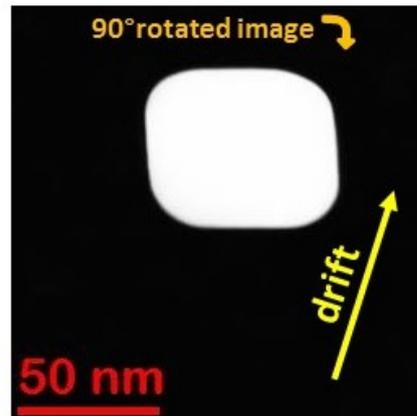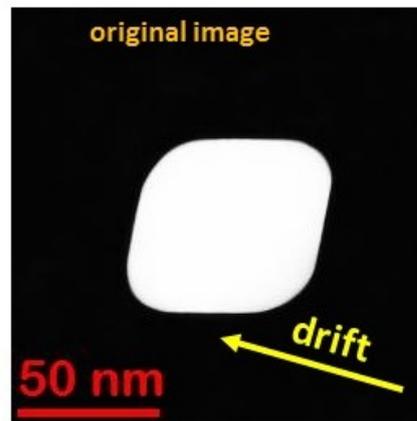
Now you have the *original* and 90°-*rotated* STEM images converted into the .dm3 format and displayed in DigitalMicrograph.
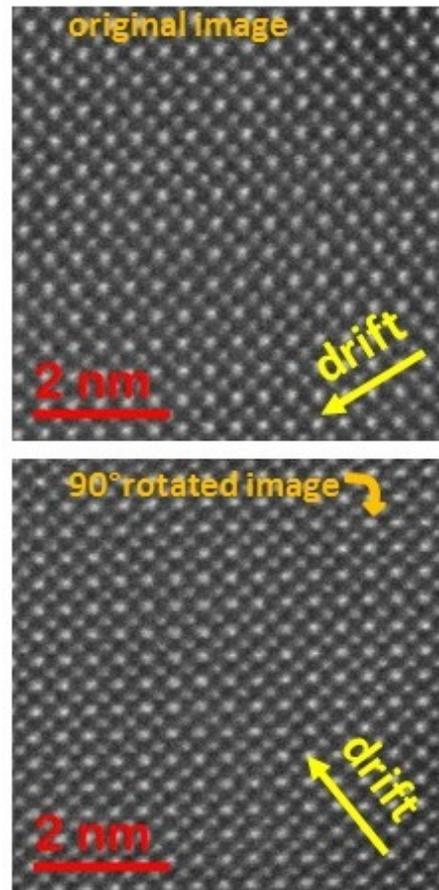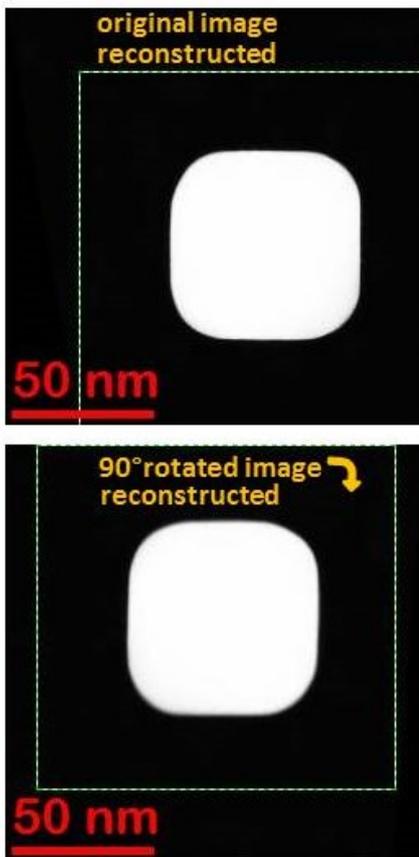
4 CROSS-CORRELATION CORRECTION OF LINEAR DRIFT

Suppose that a nanocube particle is scanned in the presence of the significant sample drift. As seen from the figure the *original* image appears distorted. You might notice the sample is drifting mainly to the left. The rotated image is distorted as well but quite differently because the drift points now mainly to the upper di-

rection. Lets try to reconstruct the real shape of the particle.

- Open the **STEMcor** tool by choosing temDM : STEMcor in the Menu.

- Click first at the *original* and then at the *rotated* image.

- Press correct drift.

The plugin performs the cross-correlation of images and deduces the direction and the magnitude of the drift (assumed constant within the course of both acquisitions). Then it warps the images in order to compensate for the distortions. Note the green rectangular ROIs in both images. They denote the areas, which are supposed to be common for both images. The out-of-

green areas cannot be correlated due to the continuous drift.

You see that the original cubic form of the particle is restored in both reconstructed *original* and *rotated* images. They appear not exactly same as the assumption of the linear drift is never perfectly fulfilled. Thus, do not try to improve statistics by averaging two images. Just use any of the restored images you like.

5 LATTICE-BASED CORRECTION OF LINEAR DRIFT

In case of atomic-resolution STEM images, the cross-correlation strategy might not work because your lattice is often essentially same everywhere. Alternatively, the drift can be measured from the distortion of the lattice geometry of both *original* and *rotated* images. Consider a next example in the figure. You see that the quadratic unit cell is slightly vertically elongated in the *original* image while compressed in the *rotated* one not mentioning the monoclinic distortion.

- Check the box lattice in the STEMcor tool.

- Click first at the *original* and then at the *rotated* image.

- Press correct drift.

The symmetry of the lattice is now noticeably improved. This is however still not a perfect lattice as the assumption of the linear drift is too simplified. The image size is retained unchanged, thus by looking at the black (out-of field) areas in its periphery you can have an idea how much the image was warped.

When the lattice is checked, the drift is estimated based on the comparison of the FFT transforms of both images. The system identifies two major reflections and then deduces the mismatch between the *original* and the *rotated* images. You can display both FFTs in order to control whether the processing is correct or not. Just hold the **SHIFT** button pressed when clicking
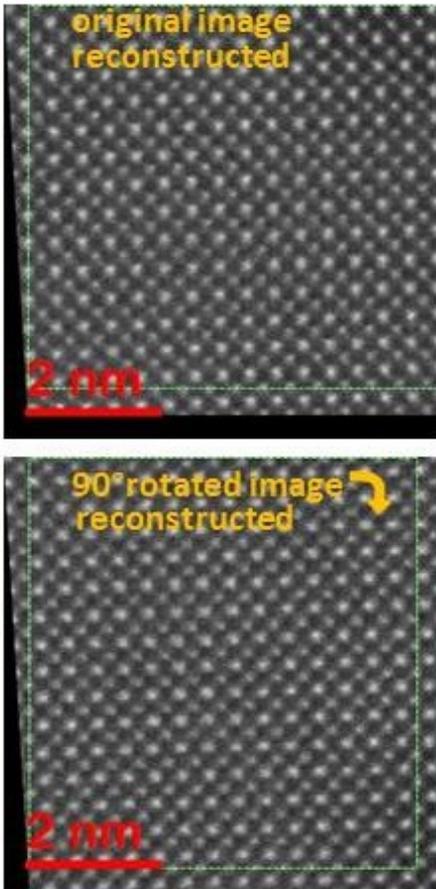
correct drift.

6 SETTINGS
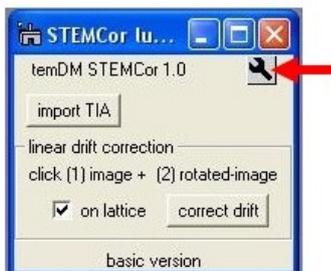
Click a spanner icon to assess the settings. First of all you can choose whether the correction using lattice will be your default option or not. This is important because people typically deal with similar kinds of images - either you mainly acquire middle mag images or atomic resolution ones. In the latter case the lattice correction must be your default, otherwise you will always forget to check the lattice box and get wrong results. The other tuned parameters define how the system treats FFT transforms. Finding lattice reflections in FFT is not a trivial task. The **temDM STEMcor** plugin first localizes the most intensive reflection and then tries to find the second strong reflection approximately orthogonal to the first one.

Range:second defines the angular range (in rad) for searching the second reflection. It must not be necessarily perpendicular to the first one. If your lattice zone possess the hexagonal symmetry the reflections will be separated by ~ 1 rad instead of $\pi/2$. Thus, it is recommended to keep this range large enough. The default value 1.2 (± 0.6 with respect to $\pi/2$) is a good value in the most cases. After the plugin identified the two reflections in the *original* image it will try to find the same reflections in the *rotated* one. They will appear at slightly different positions due to the distortions.

Range:fine is the maximal angular difference between same reflections in the *original* and *rotated* images. In fact this parameters implicitly defines the maximal allowed sample drift between two images.

The area in the very center of FFT might show quite high intensity due to the low-periodicity modulations in your image. This can make a problem for searching the strongest lattice reflections.

Radius:minK(1/nm) defines the minimal K vector (or maximal interplane distance) for the searched reflections. Effectively the area with the *minK* radius is cut-off from the FFT and will not be taken into account during the analysis.

FFT transform of STEM images are typically rather noisy. Thus, taking the maximum of the reflection does not provide the sufficient precision. The **temDM STEMcor** plugin deduces the reflection position with the sub-pixel precision by calculating the center-of-mass.

Radius:deltaK(1/nm) is the default radius in the K-space for calculating the center-of-mass of a reflection.