

# temDM STEMcor basic version

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January 1, 2020

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## 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** item 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 GET FAMILIAR WITH TEMDM TOOLS

As soon as **temDM STEMcor** is installed you can have a look at its operation tool

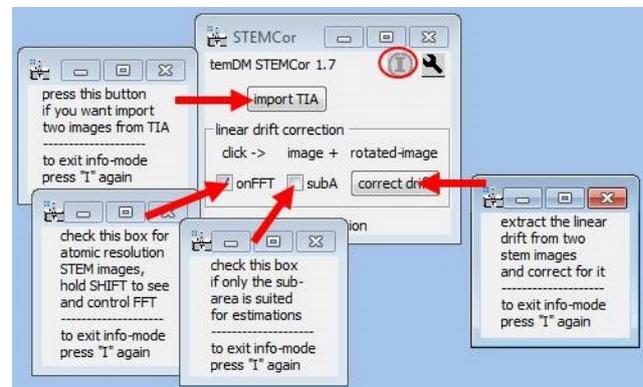
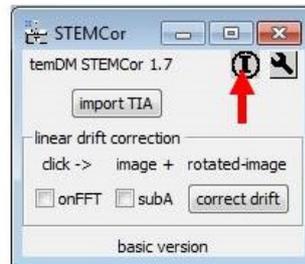
- Choose **temDM : STEMcor** in the Menu.

With this tool you can learn the basic features common for all temDM tools. They are designed for easy and comfortable operation. For instance, standard DigitalMicrographs tools are sometimes not easy to find at the workspace. They might be accidentally shifted to the the very corner of the screen or shadowed by

another tools. No such a problem for temDM tools! Try to move the **temDM STEMcor** tool around the workspace, close and open it again! All temDM tools remember their positions. Next time you open a tool, it appears exactly at the place you left it previously. So you can situate a tool at the most convenient for you position and it will be landed there in the next session.

If the position was accidentally set crazy and you cannot find it, open the tool while holding the **SHIFT** key. The tool position will be reset.

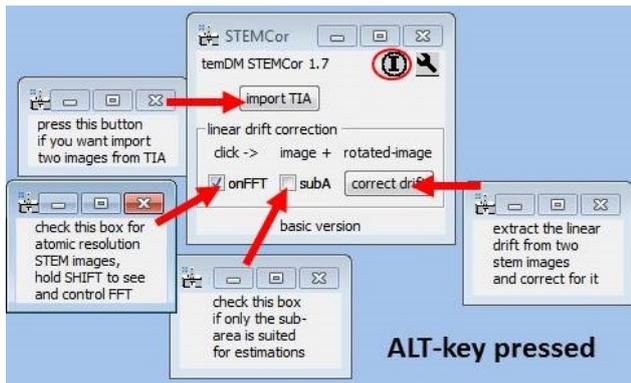
Another useful feature is a so-called information mode. You are not obliged to remember what each button is doing. Just click at the small "I" icon at the upper-right corner of the tool to activate the information mode. Now pressing any button would output a small text window explaining in short the action of a button.



Note that the "I" icon goes dim when the tool is in the information mode. To restore the normal mode just slick the "I" icon again. You can also get information about a button without activating the "I" icon. Just click the button of interest while holding the **ALT** key.

## 3 WHY STEM IMAGES NEED TO BE CORRECTED ?

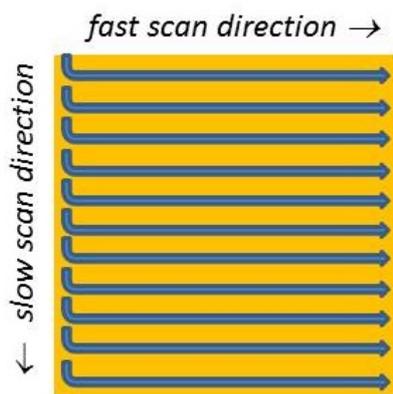
STEM stays for Scanning Transmission Electron Microscopy. Scanning implies moving the probe across the sample in order to form an image. This cannot be



proceed very rapidly and typically requires an order of magnitude longer time than shooting fixed-beam TEM images. Since different instabilities (for instance a drift of a 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 the 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 electronic) 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.

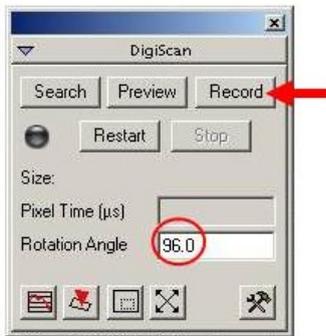
## 4 HOW TO OBTAIN TWO ROTATED STEM IMAGES

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 im-*

important to keep the minimal pause between two acquisitions.

- restore the original number in the **Rotation angle** field

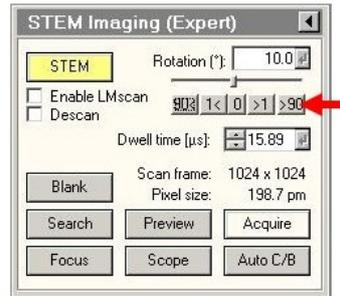
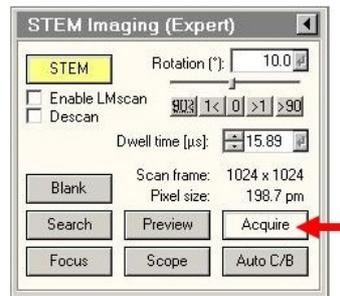


Alternatively, you can use a script for automatic acquisition of two images included in the distribution package. That would save your time and ensure the best results.

- 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.

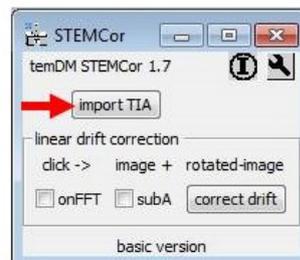
If you employ FEI TIA to collect STEM images, the action sequence is a bit more complicated.

- 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*

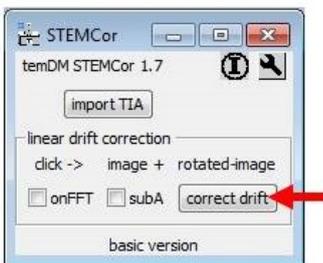
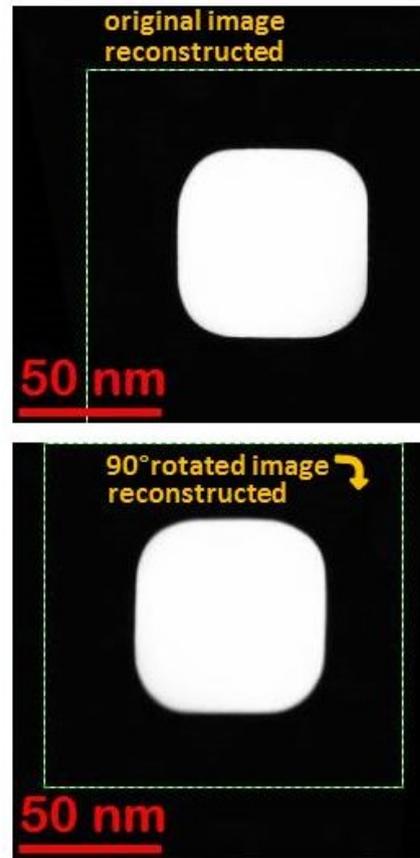
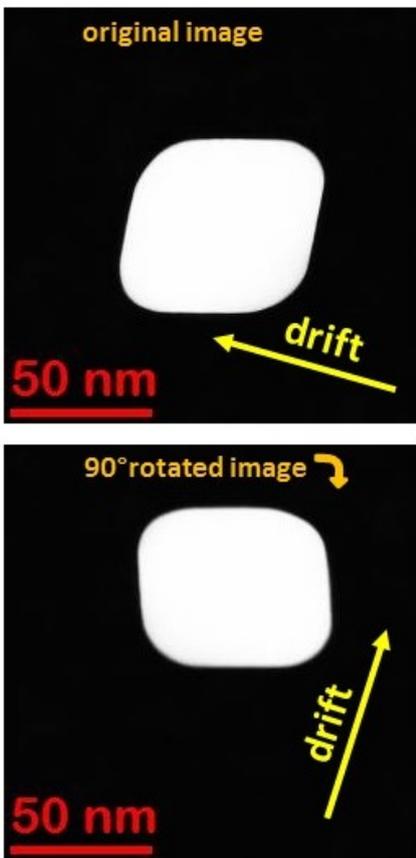


between two acquisitions.

- 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, scroll the "open" list and choose the *original* stored TIA file.
- The "open" list appears again. Choose the *rotated* stored TIA file there.



Now you have the *original* and *90°-rotated* STEM images converted into the .dm3 format and displayed in DigitalMicrograph.



## 5 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 direction. 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**.

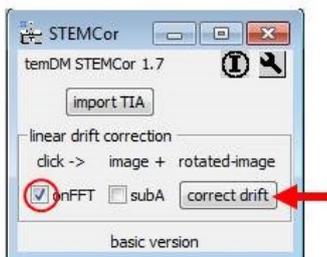
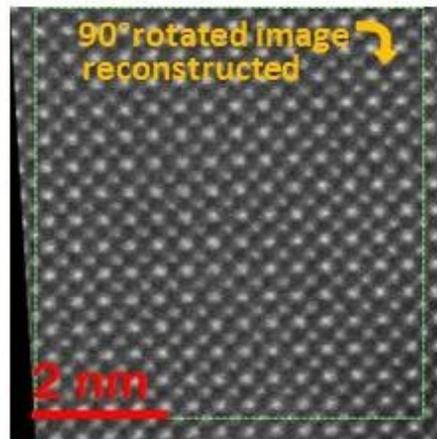
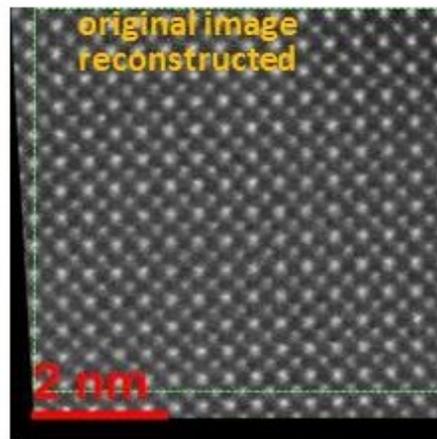
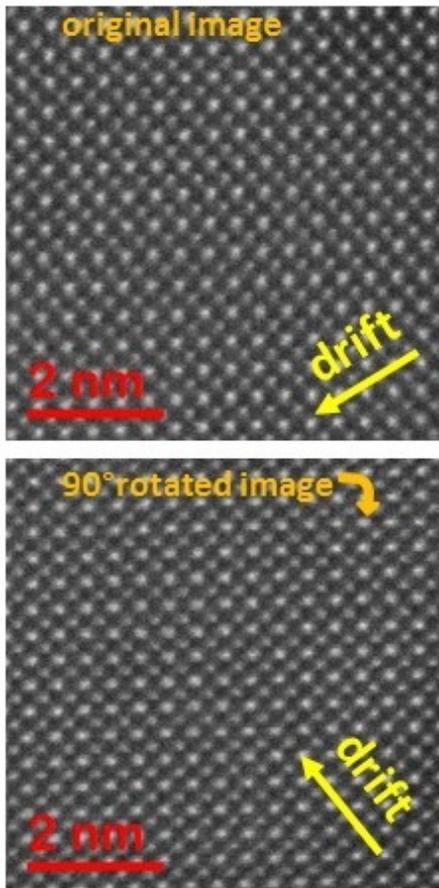
The plugin performs the cross-correlation of images and deduces the direction and the magnitude of the drift (assumed constant within the course of both acquisitions). Then it shears the images in order to compensate for the distortions. Note the green rectangular ROIs in both images. They denote the 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 however not exactly same as the assumption of the linear drift might be not very accurate.

## 6 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 the next example in the figure below. 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 **onFFT** in the STEMcor tool.
- Click first at the *original* and then at the *rotated* image.
- Press **correct drift**.

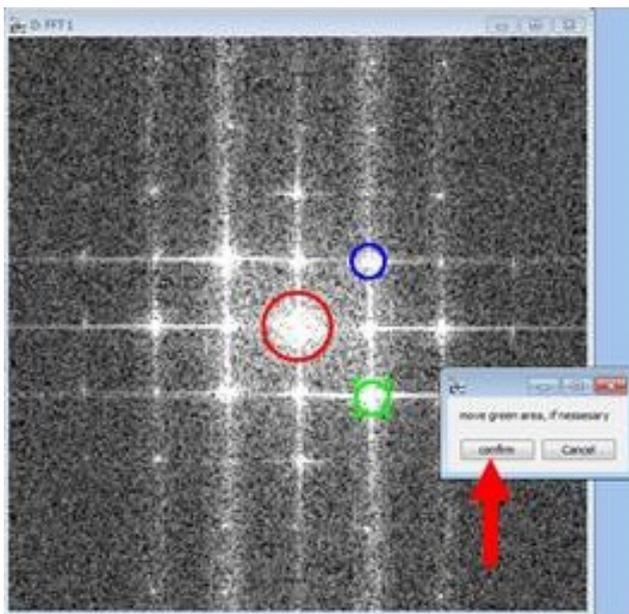
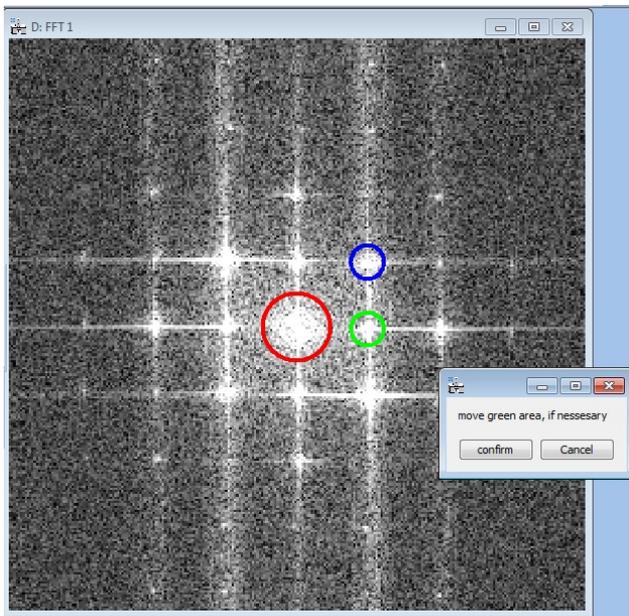
The symmetry of the lattice is now noticeably improved. This is however still not a perfect lattice as the assumption of the linear drift is too simplified. The image size is retained unchanged, thus by looking at the black (out-of field) areas in its periphery you can have an idea how much the image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

When the **onFFT** is checked, the drift is estimated based on the comparison of the FFT transforms of both

images. The plugin identifies two major reflections and then deduces the mismatch between the *original* and the *rotated* images. In some cases, the automatic finding the reflections might be not optimal. You have the possibility to control which FFT reflections are chosen and override it if necessary.

- As usual, click first at the *original* and then at the *rotated* image.
- Press **correct drift** with holding the SHIFT key.
- The FFT transform of the *original* image appears with the two major reflections outlined by the blue and green circles. For the best estimation of drift, these reflections should point to the more or less mutually perpendicular directions.
- If that is not the case (like in the shown figure) you can manually drag one of the circle to the more appropriated reflection. The only one circle (green) is moveable, another (blue) is fixed.
- Press **confirm** button.
- Similarly, the FFT of the *rotated* image should be controlled. Important: the *same* reflections

must be chosen in both *original* and *rotated* images. Otherwise the system will be confused.



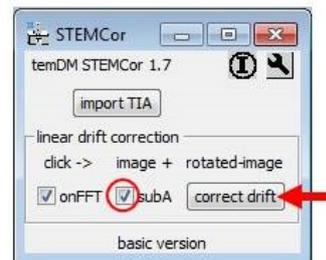
The circle should be placed only approximately on the position of the desired reflection. The exact position will be calculated as a center-of-mass within the green circle.

Please remember that the assumption of the linear drift is never perfectly fulfilled in high resolution STEM images. Thus, do not try to improve statistics by averaging two linearly corrected images. Just use any of the restored images you like. To merge two images you do need the advanced version of **temDM STEMcor** that accounts for non-linear distortions.

## 7 USING SUB-AREA FOR ESTIMATING DRIFT

Sometimes, the only part of the image is appropriated for estimating the drift. This might happen, for instance, if the image consists of both the crystalline and amorphous area and, apparently the only former is useful for the FFT analysis. In this case

- Check **subA** box and press **correct drift**.
- You are prompt to select the appropriated area in the *original* image. Press **confirm** button.

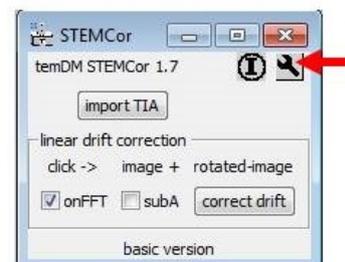


This selection should be done for the *original* image only. The selected area will be transferred to the *rotated* image automatically.

This option is available for both the FFT and cross-correlation corrections. In the latter case you might select the most recognizable feature in the image to promote cross-correlation. Please define the sub-area with a certain reserve accounting for the drift, otherwise the desired feature might drift out in the *rotated* image.

## 8 SETTINGS

Click a **spanner** icon to assess the settings.



First of all you can choose whether the correction using **FFT** will be your default option or not. This is important because people typically deal with similar kinds of images - either you mainly acquire atomic resolution images or middle-magnification ones. In

the former case the **onFFT** must be your default, otherwise you will always forget to check the lattice box and get wrong results. Similarly, you can set **subArea** default if you always treat images where the sub-area should be selected.

The other tuned parameters define how the system treats FFT. Finding reflections in FFT is not a trivial task. The **temDM STEMcor** plugin first localizes the most intensive reflection and then searches for the second strong reflection in the  $\sim$  orthogonal direction.

**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  $\sim 1$  rad instead of  $\pi/2$ . Thus, it is recommended to keep this range large enough. The default value 1.2 ( $\pm 0.6$  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.

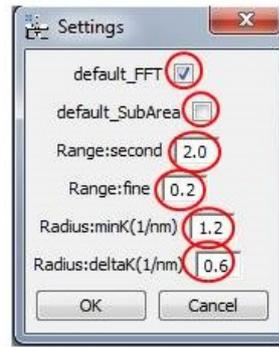
**Radius:minK(1/nm)**. The area in the very center of FFT might show quite high intensity due to the low-periodicity modulations in your image. This can make a problem for searching the strongest lattice reflections. **minK(1/nm)** defines the minimal K vector (or maximal interplane distance) for the searched reflections. Practically, the all area with the *minK* radius is cut-off from the FFT and is not taken into account during the analysis.

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

## 9 TROUBLESHOOT

*The correction looks wrong.*

Did not you exchange the *original* and *rotated* im-



ages? Please note that the *original* image should be taken first. Then the *rotated* image should be taken with a minimal pause between acquisitions. If you confuse the order, the correction will fail.

*The estimated linear drift seems to be too high. The "corrected" images look heavily sheared.*

This happens sometimes when the FFT option is used for correction. Most probably the FFT reflections are confused. Run **correct drift** with holding SHIFT key and ensure that the *same* reflections are chosen for both *original* and *rotated* images.

*The colored circles are not displayed in the FFT images. The correction is totally wrong.*

Most probably, your images are not properly calibrated. The FFT reflections are identified within some reasonable 1/nm range. This would not work for uncalibrated images.

*An error with the message "ambiguous function" is generated.*

Most probably you have loaded **temDM STEMcor.gtk** twice. Localize all Plugins folders with script **find plugins folders.s**. Only one **tem DM STEMcor.gtk** plugin must be there.

*You cannot load a temDM STEMcor tool from the menu. The tool frame does not appear.*

Last time, the tool has finish functioning incorrectly. Open the tool again with holding SHIFT key. The tool will be refreshed.

*You played too much with the temDM STEMcor settings. The program now fails or runs crazy. You have no idea what have you changed.*

Choose **New Script** in the DigitalMicrograph menu. A new text window appears. Type there **SC112\_delete()** and press **Execute**. The default settings are restored.