

temDM

temDM STEMcor

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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** in the keyboard with holding the **CNTR** key. Read the list of available plugins folders. The first folder in the list is user-specific and therefore 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. Also overwrite the plugin if you replace the basic version for the advanced one. 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_76 or
temDM STEMcor GMS3 advanced version 1_81.
```

In case you are installing the advanced version, the program will request you to input your individual installation code during the first start of DigitalMicrograph. You have to do it only once for a given PC.

2 GET FAMILIAR WITH TEMDM TOOLS

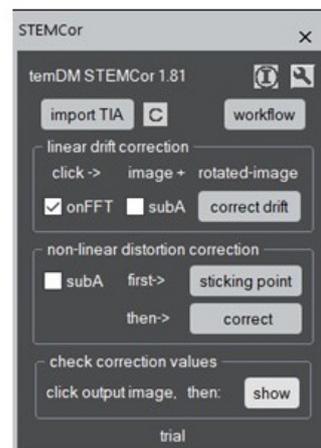
As soon as **temDM STEMcor** is installed you can have a look at its operation tool.

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

In the basic version, it looks like a small palette:



or like a larger palette in the advanced version:

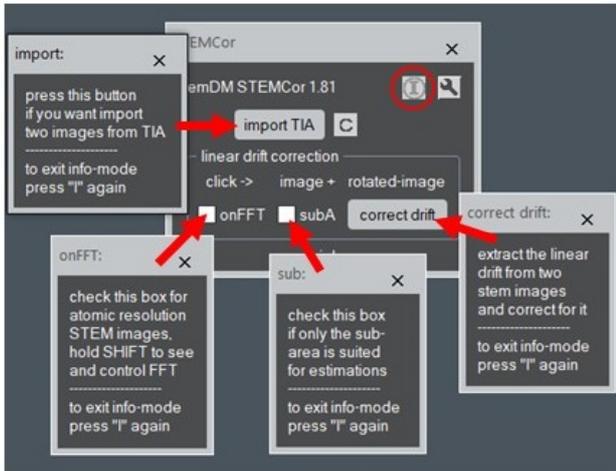


With this tool you can learn the basic features common for all temDM tools. They are designed for easy and comfortable operation. For instance, standard DigitalMicrographs tools are sometimes not easy to find at the workspace. They might be accidentally shifted to the the very corner of the screen or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

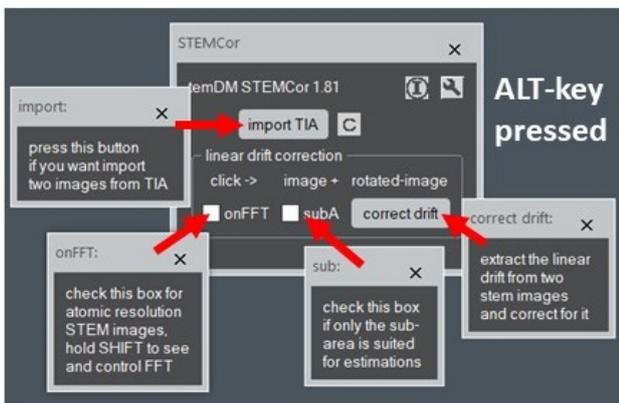
If the position was accidentally set crazy and you cannot find it, open the tool while holding the **SHIFT** key. The tool position will be reset.

Another useful feature is a so-called information mode.

You are not obliged to remember what each button is doing. Just click at the "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. The buttons are now inactive; they only deliver information about their action in this mode. To restore the normal mode just click 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.

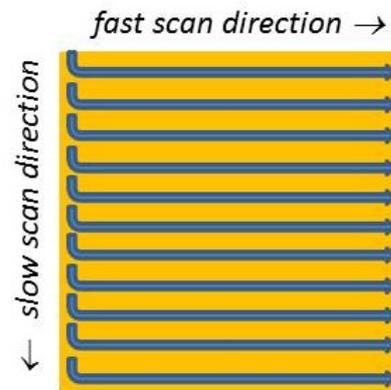


3 WHY STEM IMAGES NEED TO BE CORRECTED ?

STEM stands 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 assumedly 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** plu-

gin 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 is addressed in the advanced version of the **temDM STEMcor** plugin. The non-linear correction 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.

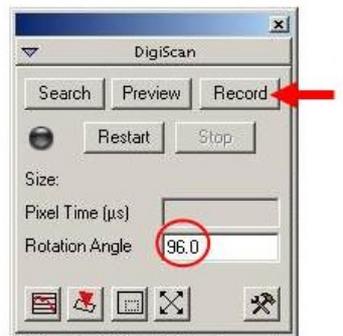
4 HOW TO OBTAIN TWO ROTATED STEM IMAGES

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** in the keyboard.
- Start the second acquisition with the **Record** button. This is going to 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 acquisition of two images included in the distribution package. That would save your time and ensure the best results.

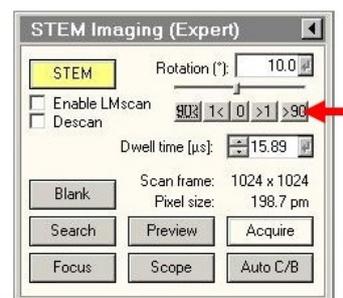
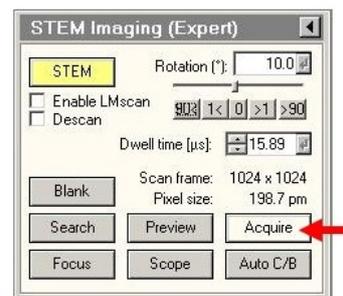
- Open **acquire (un)rotated images.s** and check the acquisition parameters - dwell time and the detector index. If you don't know to which index the desired detector is assigned, just try dif-



ferent numbers starting index 0.

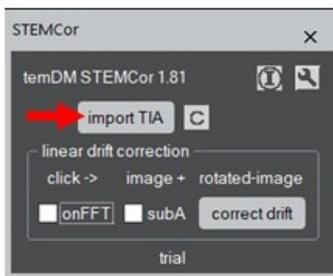
- Run the script by pressing **execute** or by pressing **ENTER** with holding the **CNTR** key.

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

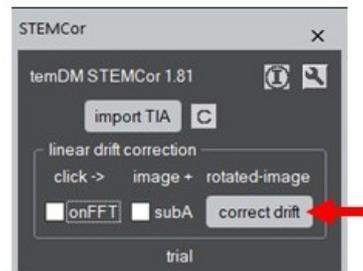
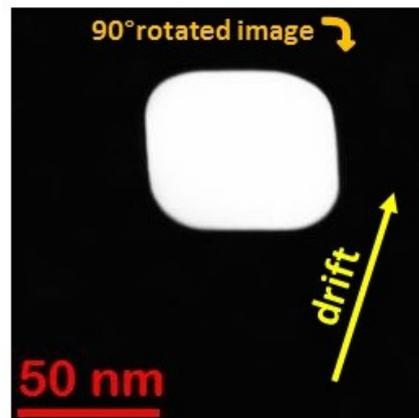
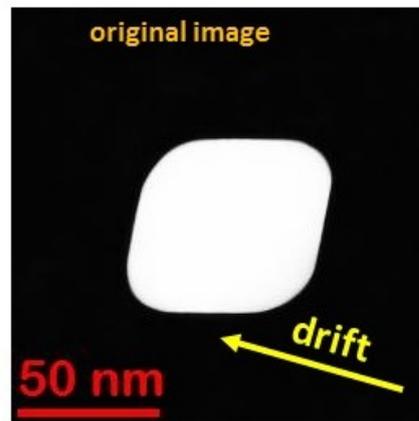


- Start acquisition by clicking **acquire** in the FEI STEM interface.

- 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

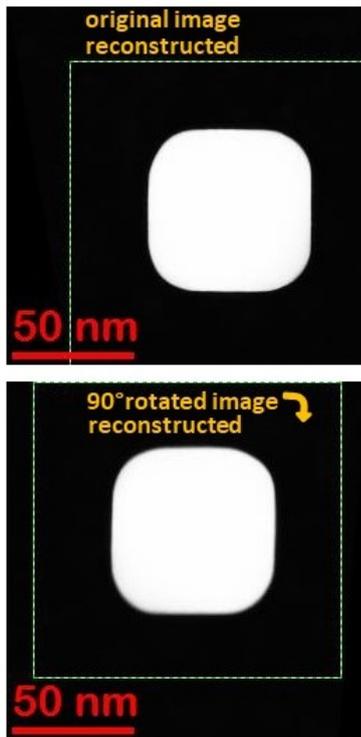
Suppose that a nanocube particle is scanned in the presence of the significant sample drift. As seen from the figure the *original* image appears distorted. You might notice the sample is drifting mainly to the left. The rotated image is distorted as well but quite differently because the drift is now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

- 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 linear drift might be not very accurate.



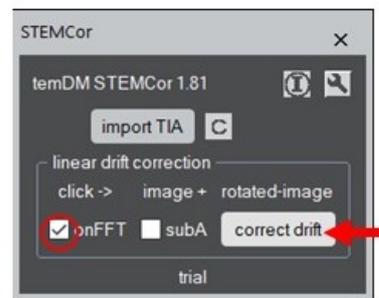
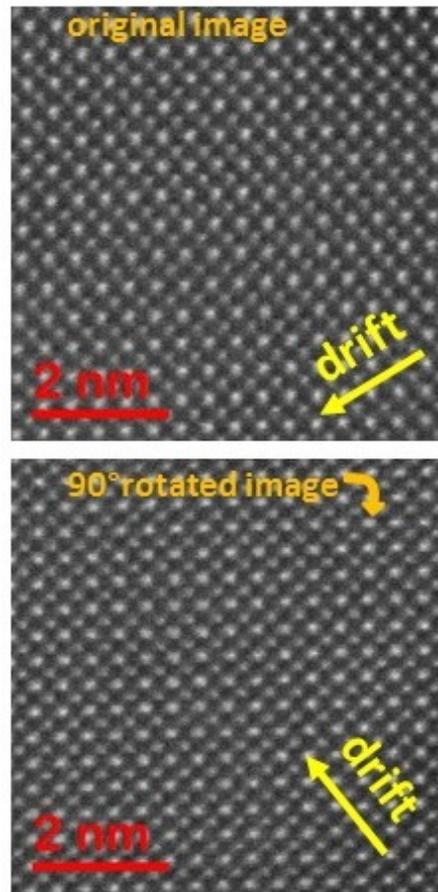
6 LATTICE-BASED CORRECTION OF LINEAR DRIFT

In case of atomic-resolution STEM images, the cross-correlation strategy typically does 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 at the top-right corner of this page. You see that the quadratic unit cell is slightly elongated vertically 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. *The sequence is important!*
- Press **correct drift**.

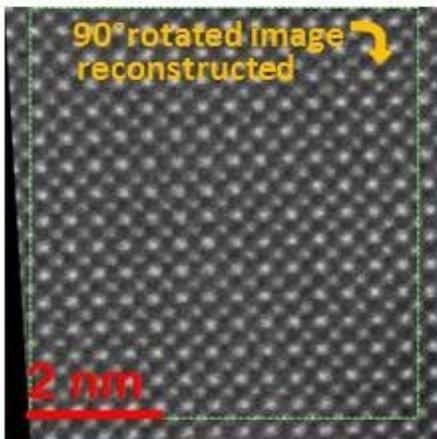
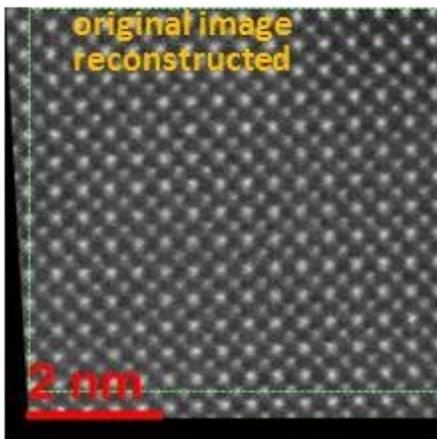
The symmetry of the lattice is now noticeably improved. This is however still not a perfect lattice as the assumption of linear drift is too simplified.

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



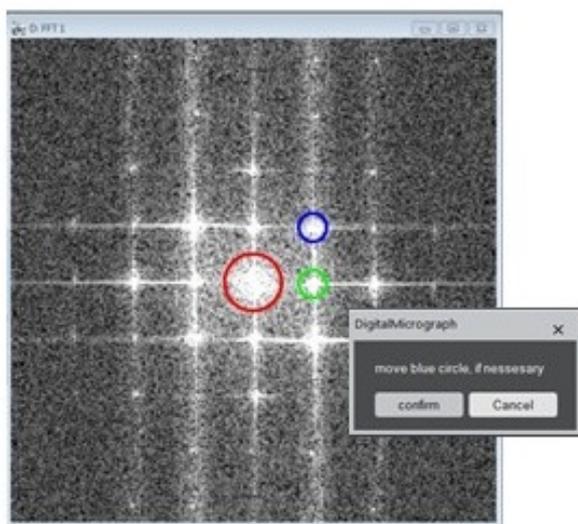
the possibility to control which FFT reflections are chosen and override it if necessary.

- 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 major reflection outlined by the **blue** circle. Usually this is the most appropriated reflection but you may drag the circle to another one you like. Press **confirm** button.
- The second reflection is outlined by the **green** circle. For best accuracy, it should point to the direction more or less perpendicular to the first one. If that is not the case (like in the figure

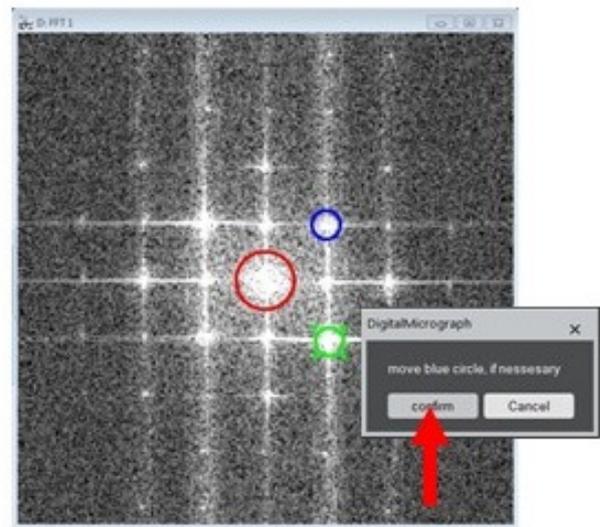


shown below) you can drag the **green** circle to the more appropriated reflection. Press **confirm** button.

- The same procedure is repeated with the *rotated* image. **Important:** the *same* reflections must be chosen in both *original* and *rotated* images. Otherwise the system will be confused.



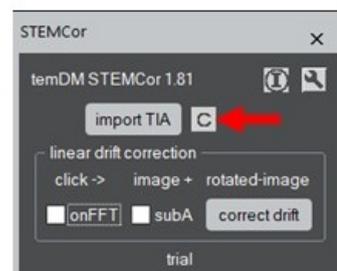
The circle should be placed only approximately on



the position of the desired reflection. The exact position will be calculated as a center-of-mass within the circles.

Please remember that the assumption of the linear drift is never perfectly fulfilled for 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.

You might notice the dark "wedge-like" areas in the corrected images. That is because the sheared image cannot fit into rectangular frame. Sometimes such areas can make a visualization problem as DigitalMicrograph might accidentally set the limits to the wrong values. Put the *initial image in back* and the *corrected image in front* and press **C** (contrast) button. The original contrast will be restored.

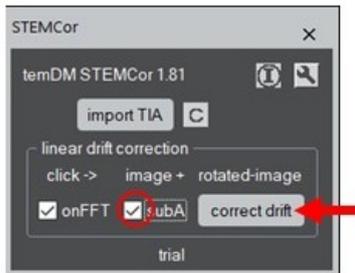


7 USING SUB-AREA FOR ESTIMATING DRIFT

Sometimes, the only part of the image is appropriated for estimating the drift. This can happen if an image,

for instance, 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 WHY NON-LINEAR CORRECTION IS NEEDED ?

The assumption of a linear drift distorting STEM images is the only first approximation. In reality, there is a lot of sources for the non-linear distortions like sudden shaking the sample, inaccuracy or instability of the scan generator and so on. These non-linearities show up clearly with increasing the magnification. In particular, atomic resolution STEM images virtually always require a non-linear correction. The figures at the top of the next page demonstrate examples of the unacceptable distortions - a sudden vertical jump (left image) or a horizontal jump (right image) between the subsequent scanned rows.

Such distortions can be however removed when analyzing a couple of images - one with the original orientation and another one with 90°-rotated scanning orientation; both images must (at least partially) cover the same area in the sample. The reconstruction can be performed after, for instance *C. Ophus et al. Ultra-*

microscopy 162 (2016) 1, who assumed that there is no distortion within any given scanned row but distortions show up as the X,Y-shifts of the rows relative their "true" positions (see the figure at the next page). If we change the direction of fast scanning, the scanned columns will be rigid while probably X,Y-shifted relative each other as shown in the figure.

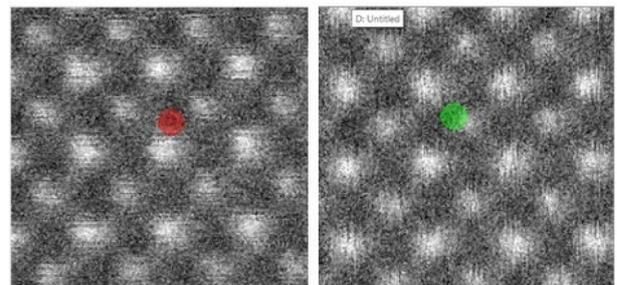
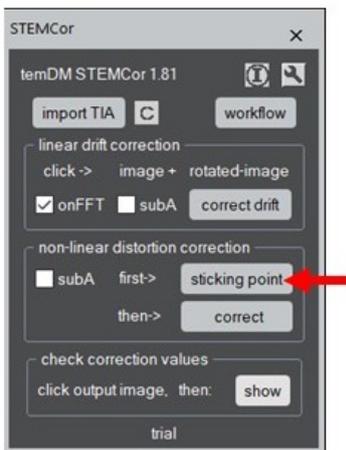
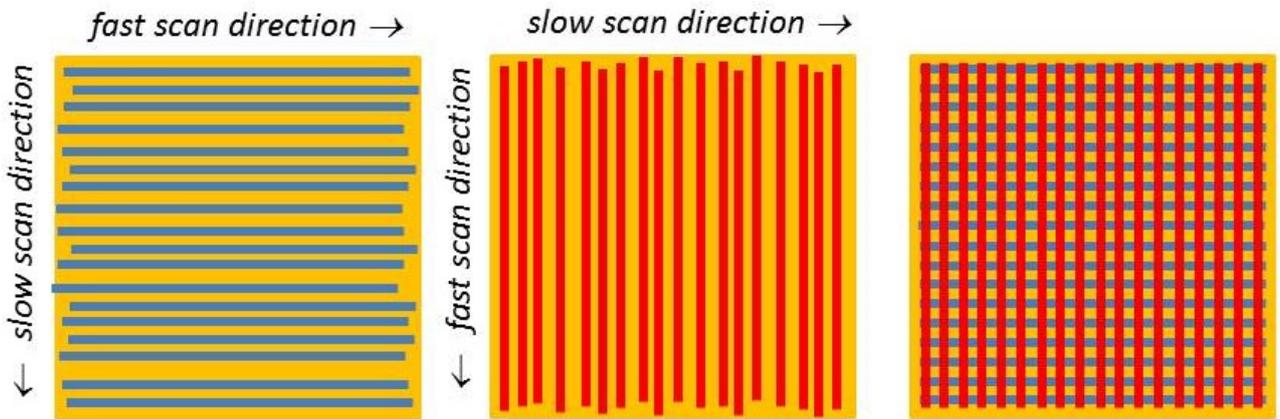
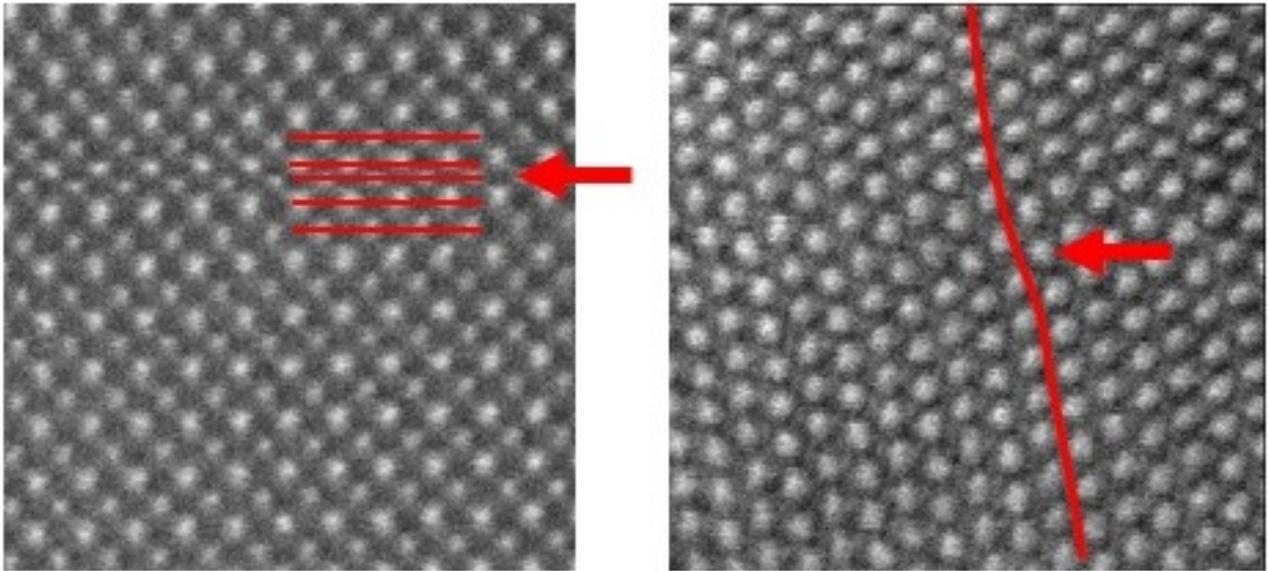
To reconstruct an undistorted image, all these shifts must be retrieved. This is a complicated but doable task. Just overlap the *original* and *rotated* images and shuffle the rows in the former and the columns in the latter until two images show the best match.

For non-linear correction you have to install the advanced version of **temDM STEMcor**. The advanced version follows conceptually the approach of Colin Ophus et al. although technically uses a rather different algorithm.

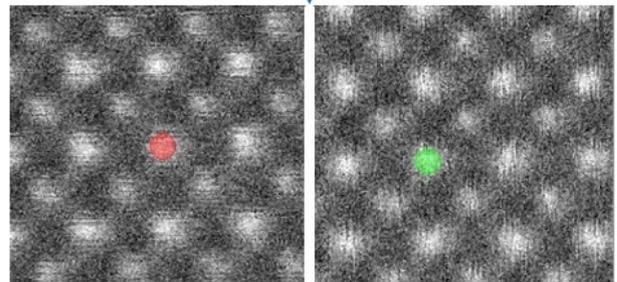
9 PREPARE IMAGES BEFORE CORRECTION FOR NON-LINEAR DISTORTIONS

Your couple of images (*original* and *rotated* orientations) should be first corrected for the linear drift. This is pre-requirement for the more advanced processing. As soon as you obtained the couple of *linearly corrected* images you can start the non-linear correction. It is an order of magnitude more complicated treatment than the linear correction, thus the system needs some minimal guideline from you. Namely, you should identify a point that you think is same in the *original* and *rotated* images.

- Having the linearly corrected *original* and *rotated* images in front press the **sticking point** button in the "**non-linear distortion correction**" box.
- You see a panel consisting of two images. The left one is your *original* image while the right one is your second image *rotated back* such as the orientation of both images is now identical.
- There are two colored markers - **red** in the left image and **green** in the right one. They are supposed to point at the position assumed to be same in both images. But initially it is never same because of the STEM distortions. First drag the **red** marker to the recognizable place in the left image. Then drag the **green** marker to the place you suppose to be same in the right image.



drag the markers such as they point to the identical atomic column



- In the floating dialog window, press **Confirm**.

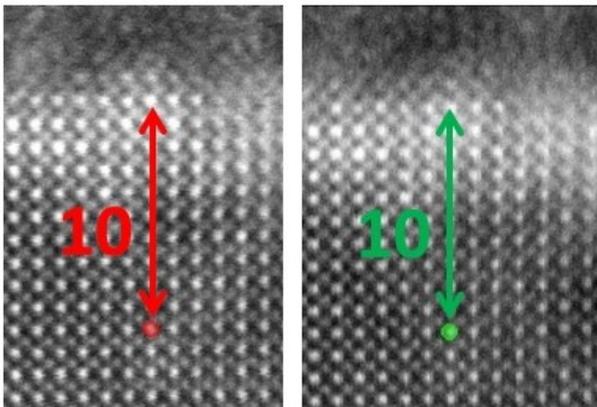
Why this is needed ? The non-linear correction is mostly applied to atomic resolution STEM images. The lattice is often composed of two or more sublattices (like in the example below), which are hard to distinguish by an algorithm. The script might easily confuse the sublattices while human eye has a greater chance

to make it correctly. Such supervision helps a lot the program and it would not take much time from you, just few seconds.

Do not afraid to mix up the original and rotated linearly corrected images (remember, it was mandatory needed to keep the right sequence before linear correction?). Now the images are internally tagged, so even if you click in the wrong order, the script knows who is who.

Setting the sticking point is user-friendly. You can zoom the images with the "loop" tool or drag it with the "hand drag" tool in order to see better the place of interest. The companion image will be displayed synchronously. *Start always with positioning the red marker* because the green marker will move accordingly. When you are sure with landing the red marker, go to the adjustment of the green one. The red marker will stay unchanged - the synchronization works only in one direction.

It is quite important to set the sticking point correctly. Note that the quality of fit might decay far from the sticking point, thus set it in the image area most important for you. Sometimes, the well recognizable features (like a defect) can be far away from the area you want to be best corrected. Then, use the following trick: count carefully the number of unit cells from the defect to your place of interest in both images and place the sticking point there.



It is not necessary to position markers very precisely. The script will refine the exact position by cross-correlation anyway. Just ensure that the required atomic column is within the red (green) marker and press **Confirm**.

Keep in mind that the program is able to correct the area not larger than 20-30 unit cells. If your image contains a larger field of view, consider correction of the smaller image part by checking box **subA** in the **non linear distortion correction** box. Then, after press-

ing **sticking point**, you can tune both the sticking point and the area (denoted by the red rectangular) to be corrected. Of course, the sticking point must be *inside* the chosen rectangular.

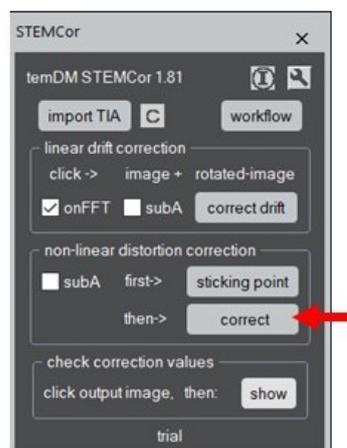


Now, everything is prepared for automatic alignment of your *original* and *rotated* images.

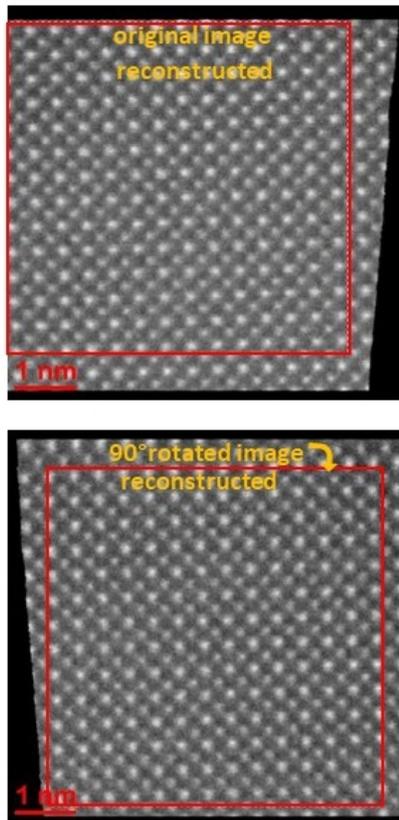
10 CORRECTION FOR NON-LINEAR DISTORTIONS

The further correction is pretty easy.

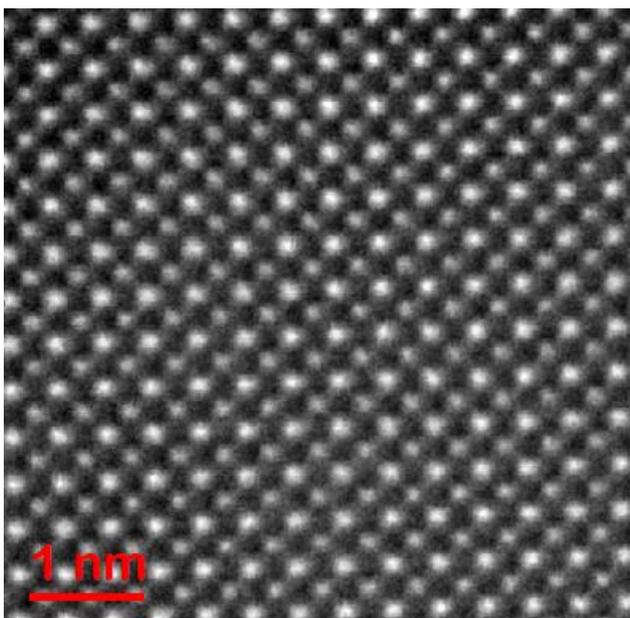
- Having the linearly corrected *original* and *rotated* images in front press the **correct** button in the "**non-linear distortion correction**" box. Wait a bit.



After the fitting procedure is finished, two new images appear - they are non-linearly corrected images in the *original* and *rotated* orientations. Red rectangular ROIs in both images indicate the calculated area of their overlap.

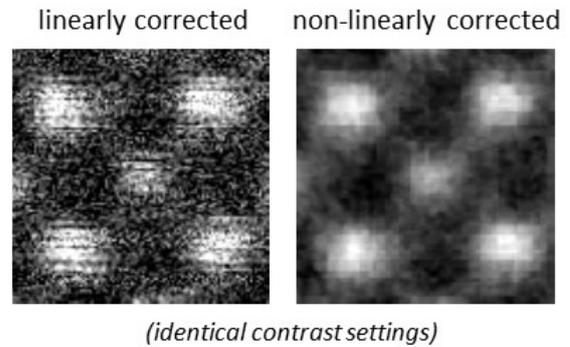


Additionally, a new image, which is combined from the *original* and *rotated* images by simple averaging within the area of overlap appears. This image will be slightly smaller in size comparing to the both input images as the overlap area is smaller than the original scan size. The combined image is calculated in the *original* orientation, not in the 90°-rotated one.



The algorithm was not specifically aimed to remove so-called STEM jitters (jagged shapes of atomic columns)

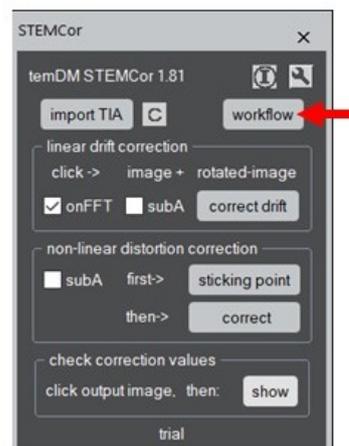
However you can notice that the jitters are significantly suppressed after the non-linear corrections. That is because the random shifts among rows are minimized, while the sporadic jumps within the rows are still present. The applied strategy results in the most reliable positioning of the atomic columns although their shapes might show some negligible jags. We however consider this as a rather cosmetic issue.



11 WORKFLOW

You might wish to make all treatments (linear + non-linear correction) as a continuous workflow.

- Just click the "workflow" button.

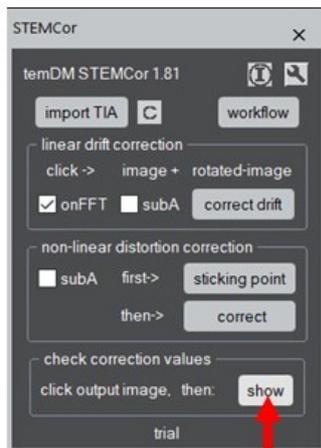


The linearly corrected images are not delivered, you will only see them when prompted to set the sticking point.

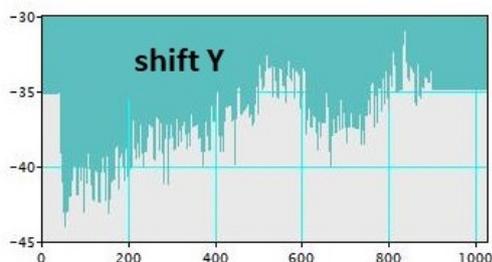
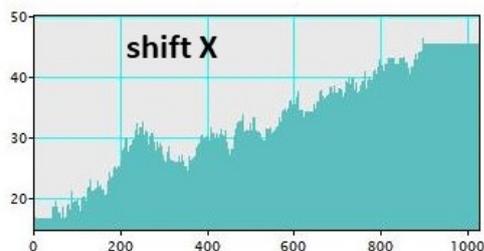
This is probably the most convenient way to work. However, if you feel some issues, turn to the step-by-step treatment (first the linear correction, then the sticking point and finally - the non-linear correction).

12 CHECK CORRECTION VALUES

At the end, you might be curious how much correction was applied to the images.



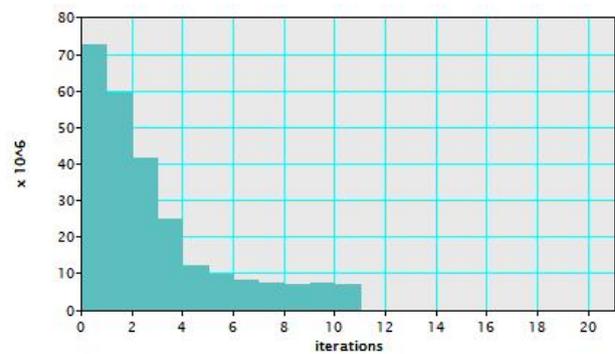
shifts applied to original image



- Having the non-linearly corrected *original* image in front press the **show** button in the "**check correction values**" box. Two plots will appear indicating the applied shifts (in pixels) for each row in the X- and Y-directions.

Do not be surprised that the shifts are flattened at the edges. There is no image overlap there, thus the shifts are assumed to be constant there and equal to the nearest available shift in the overlapped area. Similarly, the shifts applied to the columns in the *rotated* image can be extracted when having it in front.

Another kind of information is stored in the *combined* image.



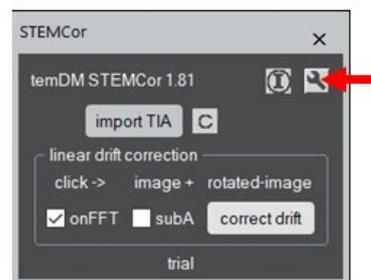
- Having the *combined* image in front press the **show** button in the "**check correction values**" box. The graphs showing convergence of iterations will appear.

The criterion of convergence in this case is the squared difference between the *original* and *rotated* images at each iteration. The fitting is executed in two stages: First, the shifts are smoothed with a cubic spline (spline correction). Second, the shifts of individual rows are varied independently (fine pixel correction). The convergence graph refers to spline correction.

The second fine correction could be not needed in many cases as it results in the only slight improvement while costs time. You can disable it through settings.

13 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.

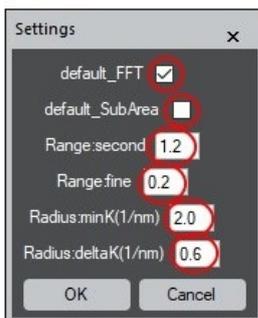
The other tuned parameters define how the system treats FFT. Finding reflections in FFT is not a trivial task. The **temDM STEMcor** plugin first localizes the most intensive reflection and then searches for the second strong reflection in the \sim orthogonal direction.

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 ~ 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 out the same reflections in the *rotated* one. They will appear at slightly different positions due to the distortions.

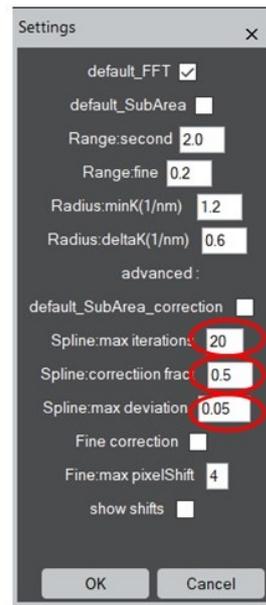
Range:fine is the maximal angular difference between same reflections in the *original* and *rotated* images. In fact this parameters implicitly defines the maximal allowed sample drift between two images.

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.



The next settings are applicable to the advanced ver-



sion and are displayed in the advanced version only.

Spline:max iterations defines the maximal number of iteration.

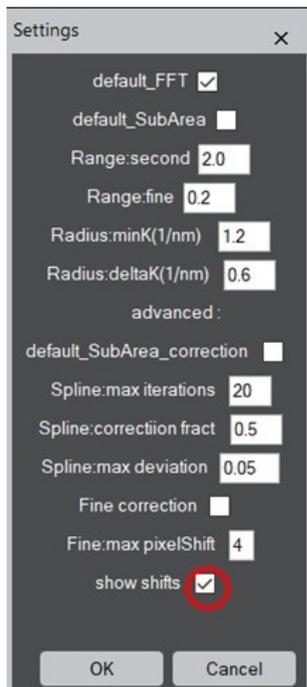
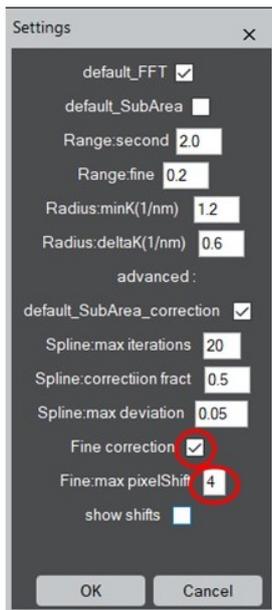
Spline:correction fract defines the value of correction applied after each iteration. It is expressed as a fraction of the measured deviation. This value should be always less than **0.5 - 0.7**, otherwise the convergence might be unstable. On the other hand, the smaller correction fraction results in longer iterations.

Spline:max deviation defines the halting criterion for iterations. Namely, when the relative difference between two subsequent iterations becomes less than this value, the iteration stops.

The next setting is relevant for the second, finer stage of fitting (when pixels are fitted independently). You can enable or disable this stage in the checkbox **Fine correction**.

Fine:max pixelShift limits the shift of rows or columns during the fine optimization. This is expressed in the number of pixels allowed to shift at each step of iteration. This number should be kept small otherwise the program might fall into the false optimum.

show shifts You might prefer to see the values of the applied shifts every time after the fitting is finished. Then, activate this option.



14 TROUBLESHOOT

The linear correction looks wrong.

Did not you exchange the *original* and *rotated* images? 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.

Your corrected image looks uncomfortably bright. The contrast seems to be distorted.

Put the *uncorrected* image in back and the *corrected* image in front and press **C** (contrast) button. The original contrast will be restored.

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.

15 REFERENCE

P. Potapov and A. Lubk. Correction for linear and non-linear distortions of STEM images, *Microsc. Microanal.* 21-S1, 2320-2322.