User Guide: STEM Moiré GPA

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1 Revision History

Date	Version	Notes
20/12/2017	1.0	First quick version

2 Symbols, Abbreviations and Acronyms

The same Symbols, Abbreviations and Acronyms as in the SRS, the TestPlan, the MG and the MIS documents (available in STEM Moiré GPA repository) are used in the User Guide document.

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3 Introduction

The aim of the document is to provide to the end user of STEM Moiré GPA some guidance to operate the software properly. The software is still under development therefore, it is very likely to find some bugs when executing the code. Considerable updates are planned to be performed nevertheless, the general use of the software should not be drastically modified. The document proposes a walkthrough of each step of STEM Moiré GPA processing using the files available in the "Examples" folder.

4 Before executing STEM Moiré GPA

The user responsibilities are described in the SRS document, nevertheless it is worth mentioning that a minimum of two files are required to execute STEM Moiré GPA which are:

- a calibrated STEM Moiré hologram (only .dm3 files are working for the moment)
- a calibrated Reference image (only .dm3 files are working for the moment)

A STEM Moiré hologram is a STEM electron micrograph in which at least one crystal periodicity is under sampled. A classic STEM electron micrograph can still be used with STEM Moiré GPA however, the software becomes a classic Geometrical Phase Analysis software.

A Reference image is an experimental STEM electron micrograph or a simulated image in which none of the crystal periodicities are under sampled. It is required, for the reference image, to represent precisely the same crystal lattice of the sample from which the STEM Moiré hologram has been acquired and preferably at its unstrained state.

One STEM Moiré hologram with its associated Reference image are present in the "Examples" folder. Those two files are going to be used in the following steps.

5 Starting STEM Moiré GPA

After downloading the source files and checking that the requirement from the dependencies are met, the main.py file can be executed and two windows should appear.Do not close these windows since there is no way of reopening them without starting the software again. The first window (fig. 1) corresponds to STEM Moiré GPA flow with all the different buttons that represent the different steps of execution which are (details of each step will be describe later in the document):

- "Input": Load the two required files
- "SMHSim": Simulate the STEM Moiré hologram from the Reference image to get the (n,m) shift for the conversion

- “GPA”: Execute the GPA algorithm to output the variation of the Moiré wave vector.
- “Ref”: Define an area of the STEM Moiré hologram as the unstrained reference
- “Convert”: Convert the Moiré wave vectors into their respective crystalline wave vectors.
- “Strain”: Calculate and display the 2D strain tensor from two non collinear crystalline wave vector.

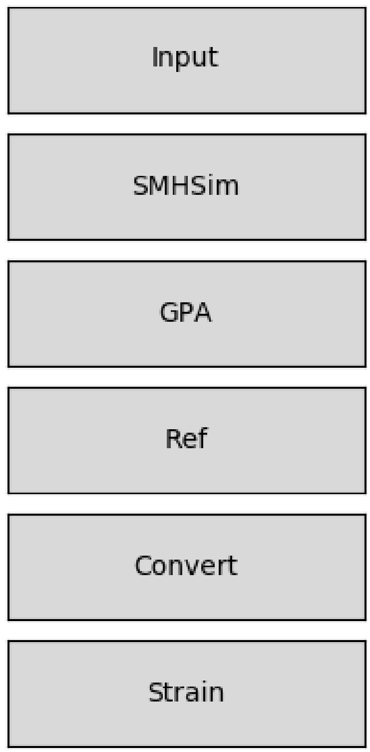

Figure 1: STEM Moiré GPA window flow

The second window (fig. 2) is composed of entry fields to let the user choose the shift to perform to convert the chosen Moiré wave vector to its corresponding crystalline wave vector. Only integer numbers are accepted in the entry field.

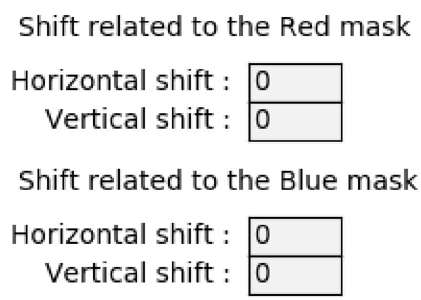

Figure 2: Conversion window

6 Load files

To load the required files, select the "Input" button in STEM Moiré GPA window flow. A dialog will appear (fig. 3) requesting you to choose first the STEM Moiré hologram and then the Reference image. An error message should appear if the loading process was not performed properly. At the end of the loading process a new window with the STEM Moiré hologram and reference image should appear (fig. 4)

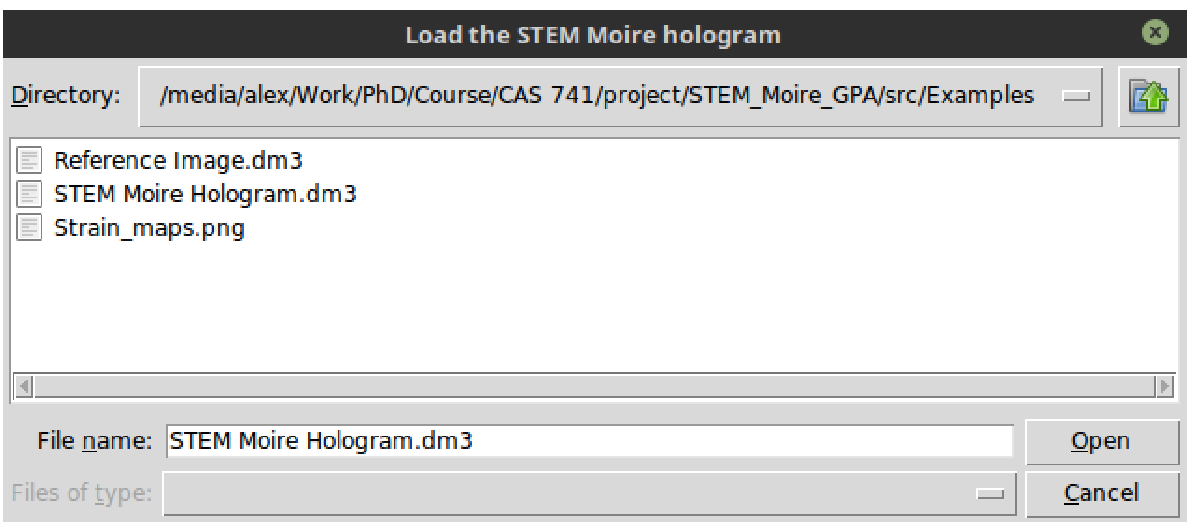

Figure 3: Load file dialog

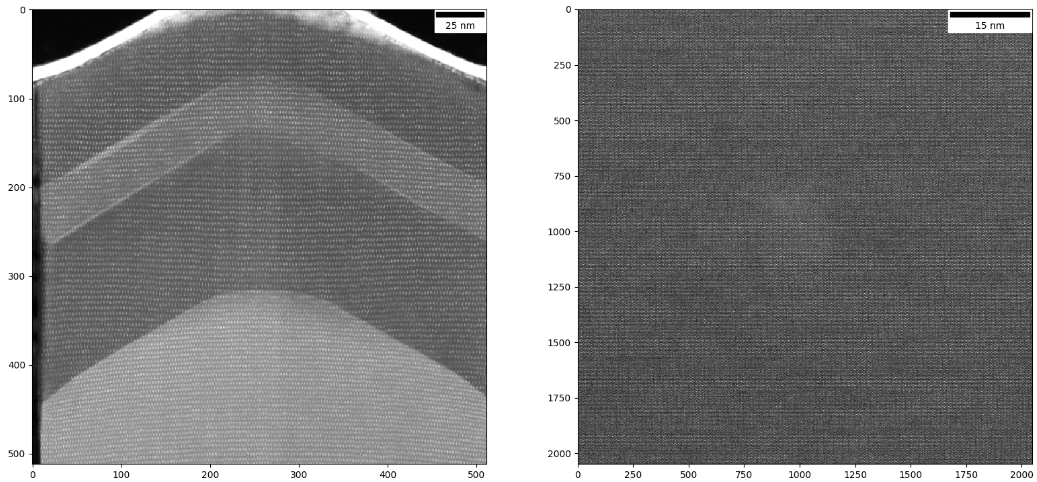

Figure 4: STEM Moiré hologram and reference image window

7 Simulate the STEM Moiré hologram

Once the files loaded, select the “SMHSim” button to launch the simulation process. Please be patient, this step can take some time. At the end of the simulation, three windows will appear:

- the “SMH simulation window” fig. 5: this is the most important window and should not be closed at any time since it is used in the next steps of STEM Moiré GPA processing. On the left image is presented the Fourier Transform of the experimental STEM Moiré hologram with a red and a blue circle (their role will be describe later). On the right image is shown the Fourier transform of the simulated unstrained STEM Moiré hologram from the reference image. The user should be able to identify some correspondence between the two images (position and arrangement of the reflections). If it is not the case, the reference image is probably inappropriate.

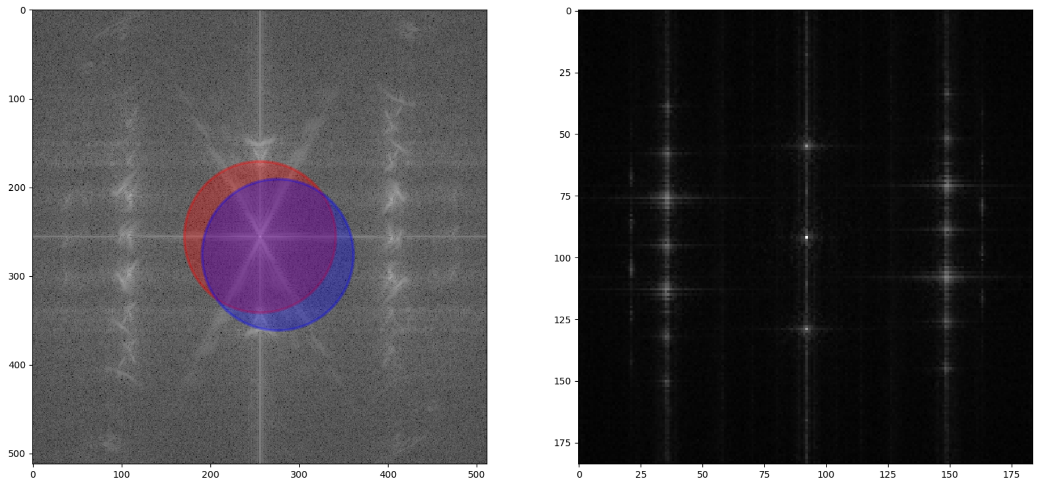

Figure 5: STEM Moiré hologram simulation window

- the “SMH Simulated with colors” (fig. 6): this window follows the same color code as “Ic split into tiles” and represents the Fourier transform of the simulated STEM Moiré hologram. It is the identical version of the one present in the “SMH simulation window” but with colors and more noise. The colors are here to help in distinguishing the different reflections.

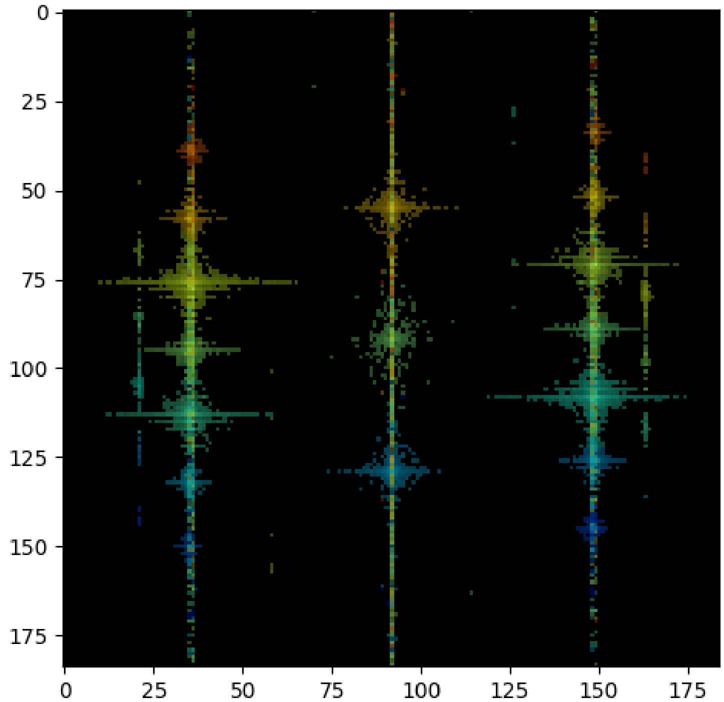

Figure 6: STEM Moiré hologram simulated with colors window

- the “Ic split in tiles” (fig. 7): this window needs to be read in parallel with “SMH Simulated with colors” and represents the effect of sampling on the reference image. The separation in tiles with different colors is to make the link between the reflection position in enquoteSMH Simulated with colors and the tiles they originate.

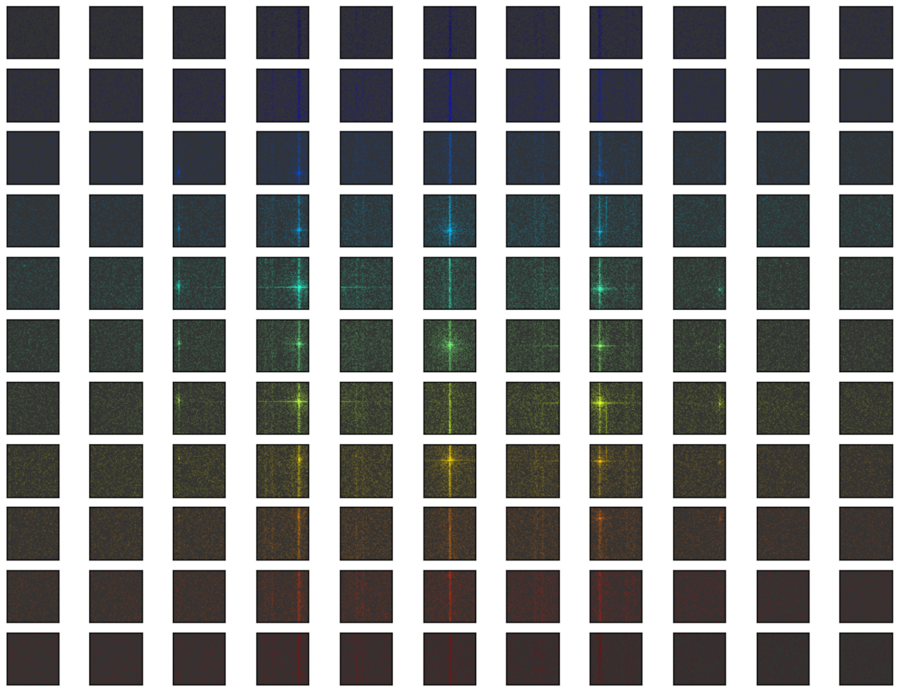

Figure 7: Reference image split in tiles window

The goal of the simulation step is to read the necessary shift to convert the Moire wave vector into the crystalline wave vector. Figure 8 is summarizing the sampling process and the shift effect on the tiles (some notion of crystallography is advised to interpret the data). The sampling effect can be imaged by considering the overlap (or the sum) of each individual tile into the central tiles. Taking for example the tile g_{0002} circled in blue in fig. 8, a "(-2,0) shift" (2 vertical shift down and 0 horizontal shift) brought by the undersampling condition, is adding the contribution from the g_{0002} tile into the central tile. The contribution on the central tile of the g_{0002} tile can be found on the Fourier transform of the simulated STEM Moiré hologram (right image in fig. 8) by finding the corresponding color. The same methodology can be applied for the g_{1-100} tile circled in green. In this case a "(0,-2)" shift is generated by the undersampling condition to add the contribution of the g_{1-100} tile in the central tile.

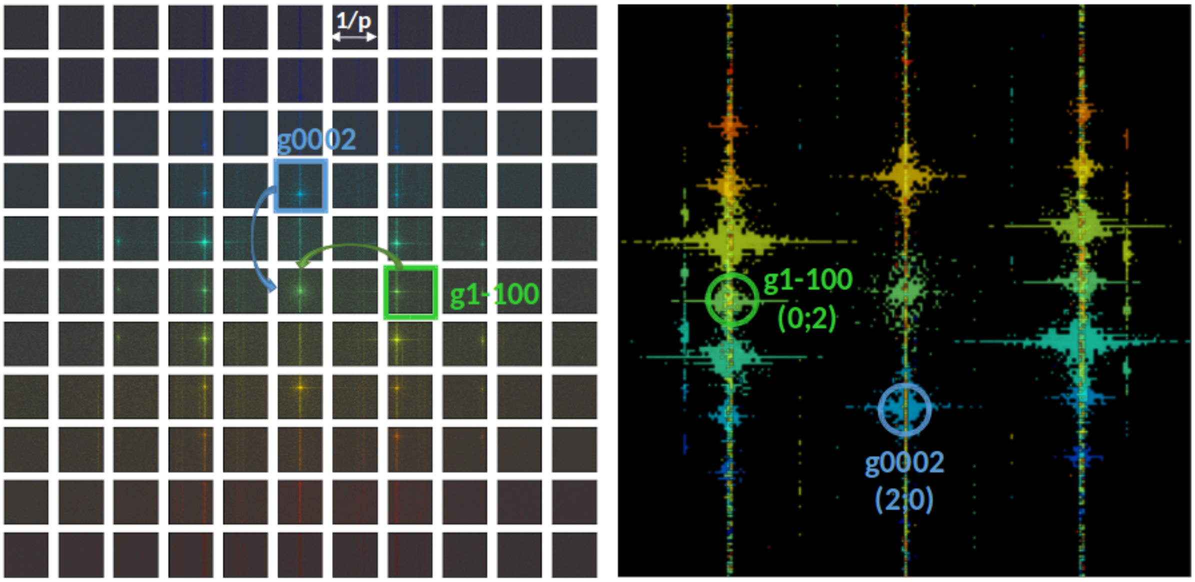

Figure 8: Extract the shift from the simulation data. On the left is shown the reference image split in tiles and on the right is shown the Fourier transform of the simulated STEM Moiré hologram.

The two shifts identified and their contribution localized in the Fourier transform of the **simulated** STEM Moiré hologram, the correspondence can be done on the Fourier transform of the **experimental** STEM Moiré hologram. An example is shown in fig. 9 where corresponding reflections are first identified on the experimental data (by analogy with the simulated one). Then, to compensate the undersampling effect, the opposite shifts compared to the ones earlier identified need to be considered to recover the original signal from the crystal. Therefore, the shift, for the conversion process, for the g_{0002} reflection will be (2,0) (Shift vertical = 2 and shift horizontal = 0) and (0,2) for the g_{1-100} reflection (Shift vertical = 0 and shift horizontal = 2). These sets of shifts are the ones that are going to be used to fill the entry fields of the conversion window (fig. 2) before executing the conversion process.

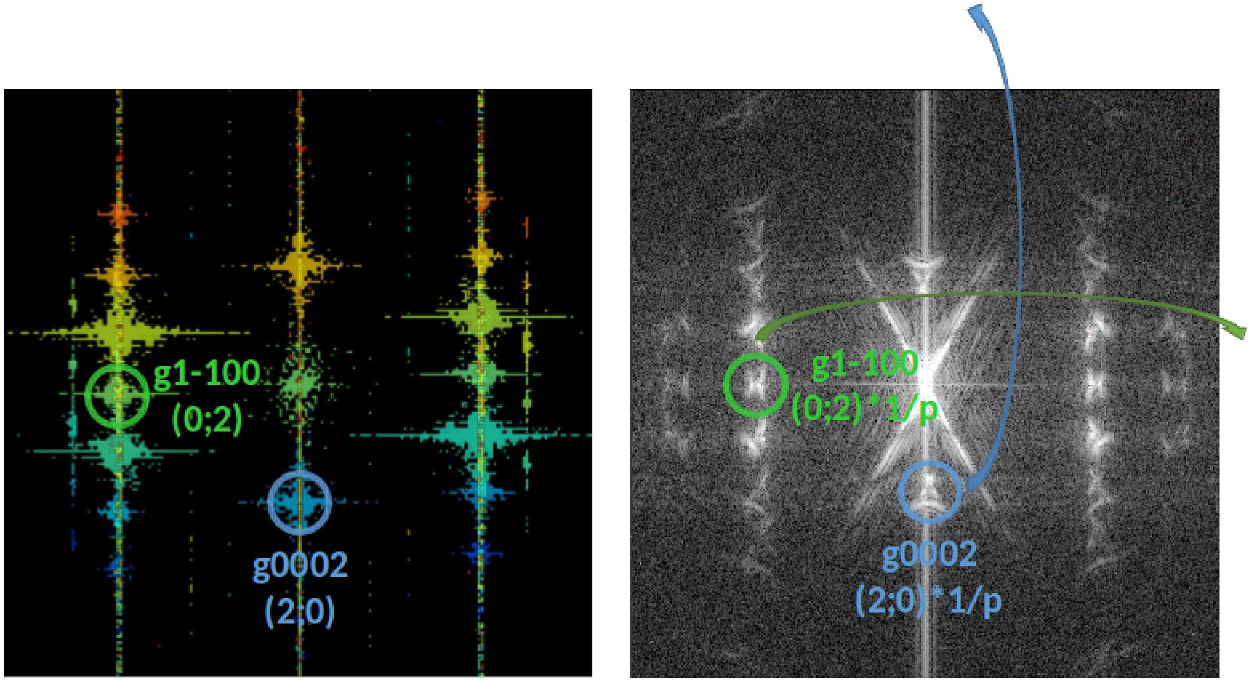

Figure 9: On the left is shown the Fourier transform of the simulated STEM Moiré hologram and on the right the Fourier transform of the experimental STEM Moiré hologram.

Once the shift determined, the “Ic split in tiles” and the “SMH Simulation with colors” windows can be closed. Those won’t be reused in the following steps.

8 Apply the GPA algorithm

With the GPA algorithm, the user wants to isolate a particular spatial frequency to capture the variation of the wave vector. With the previous step, the user should have identified two non collinear reflections in the Fourier transform of the experimental STEM Moiré hologram. Those two reflections are the ones that are going to be selected using the red and the blue circle available in the window. The position and the radius of the circles will define the mask that are going used by the GPA module.

To edit the position and the radius of both circles, the user should press the letter "e" on the keyboard (while having the “SMH simulation window” fig. 5 active) to toggle the editing mode of the window. Then, select the circle with the left click to position it on the selected reflection and modify the radius using the right click of the mouse. The position and the radius of the circles have non negligible effects on the performance of the GPA algorithm (resolution and sensitivity). The effects are described in the Test Report document and should be use as recommendations to find the proper conditions. Once the circles are positioned properly (by isolating respectively one isolated feature only), the user should press the letter "d" to lock the properties of the circles and turn off the edit mode.

If needed the user can press "e" again to turn on the edit mode. When the modification finished, it is mandatory for the user to turn off the editing mode for the GPA function to be executed.

Figure 10 is an example of what a user should get after editing the position and the radius of the circles. It is possible to note that one circle is filled and the other one is unfilled. The difference is to identify the circle that has been selected for the GPA process. The selected mask is the one which is unfilled.

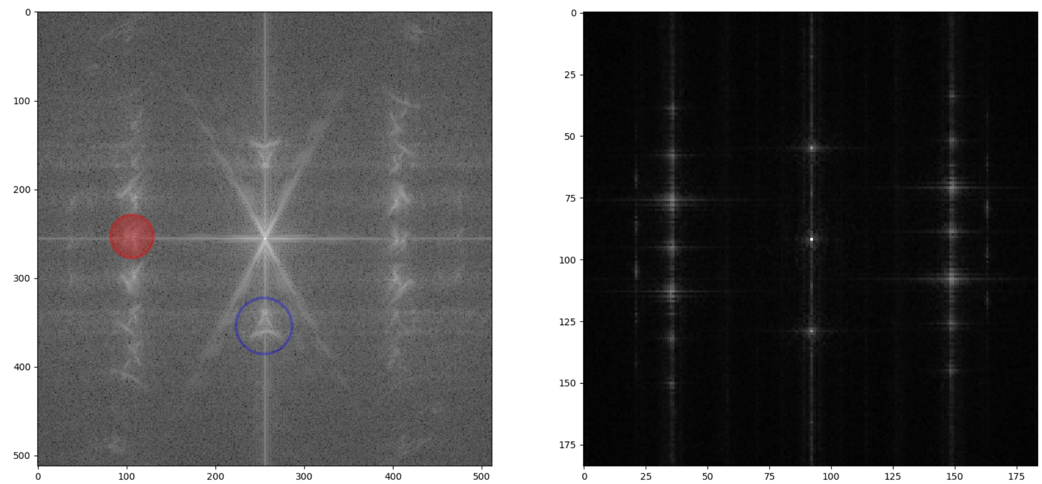

Figure 10: STEM Moiré hologram simulation window with the mask positioned

Once the circles drawn, select one by clicking on it and select “GPA” button to execute the GPA algorithm on the selected mask. A new window will appear (fig. 11) representing the phase variation and green rectangle to choose an unstrained reference on the image. It is advised to execute the GPA algorithm on the other mask also by selecting the other mask in the “SMH simulation window” (fig. 5) before selecting the reference in the next step. With both phase images displayed, the reference will be automatically adjusted for both images at once.

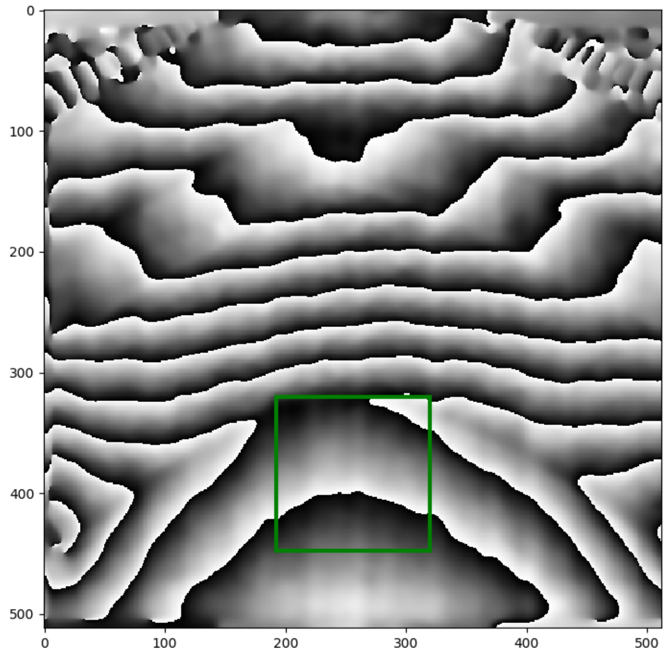

Figure 11: Phase image from the blue mask using the GPA algorithm

9 Define the unstrained reference

With both phases images displayed, it is possible to define an unstrained reference on the either of the phase images by drawing a rectangle on where the reference is supposed to be. The draw process correspond to a first right click to define the top left corner of the rectangle and drag the mouse to the bottom right corner of the rectangle and release the mouse button. Once the area define, select the button "Ref" to update the unstrained reference and the phase images. The reference definition should update the phase like in fig. 12.

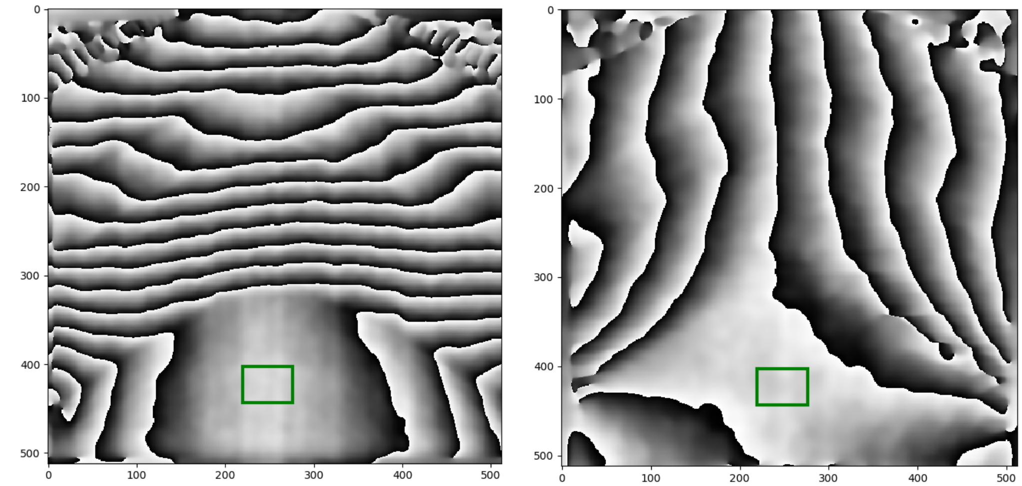

Figure 12: Updated phase images with the unstrained reference defined. The left image corresponds to the blue mask and the right image corresponds to the ref mask.

10 Convert the Moiré wave vector into crystalline wave vector

The shifts for each chosen reflection (covered by either the blue or red masks) have been chosen from the STEM Moiré simulation process. The shifts have to be manually implemented into STEM Moiré GPA to perform the conversion. A (2,0) shift has been identified for the g_{1-100} reflection (red mask), so an horizontal shift of 2 and a vertical shift of 0 should be written in the appropriate entry fields. A (0,2) shift has been identified for the g_{0002} reflection (blue mask), so an horizontal shift of 0 and a vertical shift of 2 should be written in the appropriate entry fields. For the example described here, the conversion input window should like in fig. 13.

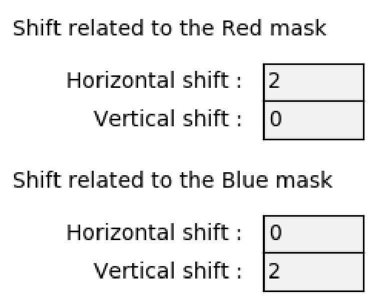

Figure 13: Updated phase images with the unstrained reference defined. The left image corresponds to the blue mask and the right image corresponds to the ref mask.

Once the shift values inputed, select the button “Convert” to perform the conversion. When the conversion is done, a message appears in the terminal.

11 Calculate the 2D strain tensor

Once the conversion performed, select the button “Strain” to perform the strain calculation. Each element of the 2D tensor is displayed as a map highlighting the uni-axial strain along the horizontal and the vertical direction, the shear strain and the rotation. All the 4 maps a regrouped in one figure as shown in fig. 14.

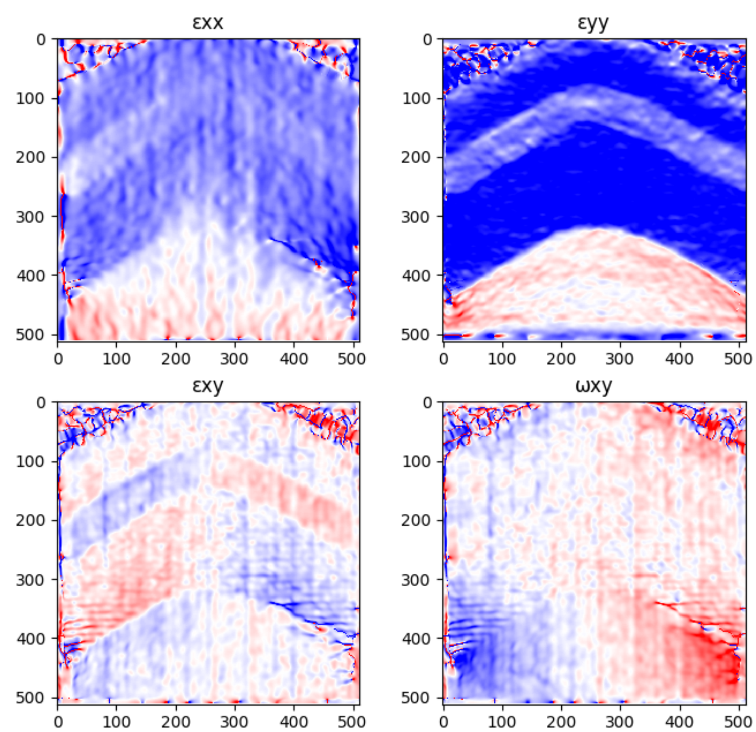

Figure 14: Updated phase images with the unstrained reference defined. The left image corresponds to the blue mask and the right image corresponds to the ref mask.

With the strain maps the flow of STEM Moiré GPA is completed. New features will be added to manipulate the data in a future release (change contrast, change color map, perform a line profile, ...). The user guide will be accordingly updated once the new functions are implemented.