

June 2017

*STEM Moiré Analysis  
(sMoiré)  
for DigitalMicrograph*

*Analysis of STEM digital moiré images  
for Strain Mapping*

STEM Moiré Analysis (sMoiré): v1.3.1

HREM Research Inc.

## Conventions

The typographic conventions used in this help are described below.

<b>Convention</b>	<b>Description</b>
<b>Bold</b>	Used to denote components of the user interface such as buttons, field names, menus, and menu options. For example, the <b>New</b> button.
<b>Menu...MenuOption</b>	Select the menu from the menu bar then select the menu option from the menu. For example, <b>File...Open</b> would mean to select the <b>File</b> menu and then the <b>Open</b> option.
CAPS	Used to denote the name of a key on the keyboard. For example, the ENTER key.
<i>Italics</i>	Used to denote emphasis, captions and the result of an action in a procedure.

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Portions of this document were prepared by HREM Research Inc. by editing the materials supplied by Dr. Martin Hytch.

DigitalMicrograph is a trade mark of Gatan Inc.

## Software requirements

The following is a list of the software requirements necessary to run the sMoiré plug-in:

- DigitalMicrograph (GATAN™)
- USB Key Driver
- HREM Mouse Tool Plug-in (Free-ware downloadable from [www.hremresearch.com](http://www.hremresearch.com))
- IPU Plug-in (Free-ware downloadable from [www.hremresearch.com](http://www.hremresearch.com))

## Software Installation

### Installing USB Key Driver

The user key driver should be installed by following the instructions given by the key driver installer. The key driver installer comes with sMoiré, or you can find it on our web site.

### Installing sMoiré Plug-in

The plug-in can be installed by drag-and-drop copy to the folder “PlugIns” (The PlugIns folder should exist under a normal installation of the DigitalMicrograph.)

When the DigitalMicrograph is launched after placing the plug-ins into the PlugIns folder, sMoiré menu commands will appear under “sMoiré” menu.

### Installing Mouse Tools

All the files relating Mouse tool plug-in can be installed by drag-and-drop copy to the folder “PlugIns.” (The PlugIns folder should exist under a normal installation of the DigitalMicrograph.)

When the DigitalMicrograph is launched after placing the plug-ins into the PlugIns folder, the Mouse tool will appear as an addition to the standard tools.

### Installing IPU Plug-in

sMoiré uses some functions based on the Intel’ MKL (Math Kernel Library) provided by the IPU plug-in. All the files relating the IPU plug-in can be installed by drag-and-drop copy. Please consult the ReadMe file that comes with the IPU plug-in.

# Introduction to STEM Moiré Analysis

Welcome to the STEM Moiré Analysis plug-in for DigitalMicrograph, or sMoiré for short. The software provides the analysis for creating strain maps from scanning transmission electron microscope moiré fringes (SMF).

Artificial moirés are created in a STEM by deliberately choosing a low magnification where the high-resolution image is undersampled and the scan step is close to the crystalline periodicity. A moiré contrast then results from the interference between the scan and the crystal lattice. The idea, which has been applied to many kinds of scanning microscopy techniques, was first proposed for STEM in the following publication:

- [1] D. Su and Y. Zhu, **Ultramicroscopy** 110, 229–233 (2010). *Scanning moiré fringe imaging by scanning transmission electron microscopy*. [10.1016/j.ultramic.2009.11.015](https://doi.org/10.1016/j.ultramic.2009.11.015)

The technique was further developed to analyse strain:

- [2] S. Kim, Y. Kondo, K. Lee, G. Byun, J. J. Kim, S. Lee and K. Lee, **Applied Physics Letters** 102, 161604 (2013). *Scanning moiré fringe imaging for quantitative strain mapping in semiconductor devices*. [10.1063/1.4803087](https://doi.org/10.1063/1.4803087)

and was applied to the study of strained-silicon devices in a follow-up paper:

- [3] S. Kim, Y. Kondo, K. Lee, G. Byun, J. J. Kim, S. Lee and K. Lee, **Applied Physics Letters** 103, 033523 (2013). *Quantitative measurement of strain field in strained-channel-transistor arrays by scanning moiré fringe imaging*. [10.1063/1.4816286](https://doi.org/10.1063/1.4816286)

The spacing and orientation of the moiré fringes can be related to the strain in the sample. In this package, we extract this information using the concept of geometric phase, previously used for the analysis of high-resolution TEM images:

- [4] M. J. Hÿtch, E. Snoeck, R. Kilaas, **Ultramicroscopy** 74 (1998) 131–146. *Quantitative measurement of displacement and strain fields from HREM micrographs*. [10.1016/S0304-3991\(98\)00035-7](https://doi.org/10.1016/S0304-3991(98)00035-7)

The advantage of this formulation is that the moiré fringes do not need to be aligned exactly with the crystalline lattice, thus freeing up the experimental work.

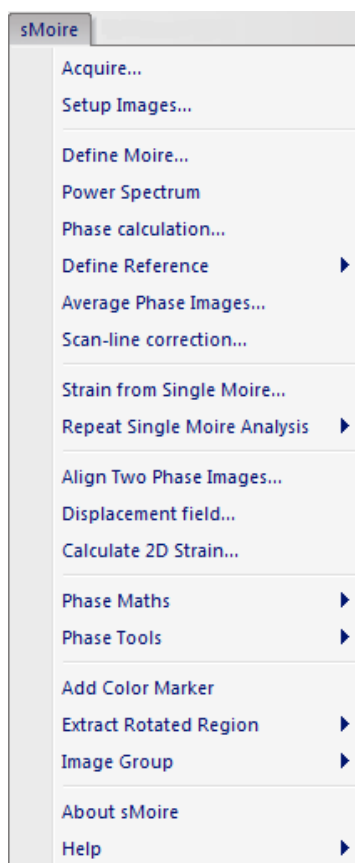
The procedure to determine the two-dimensional strain maps from two differently oriented SMFs was developed based on the procedure developed for HoloDark (the *DigitalMicrograph* plug-in for strain analysis using Dark-Field Holography):

- [5] M.J. Hÿtch, F. Houdellier, F. Hüe, and E. Snoeck, *Nature* 453 (2008) 1086-1089. Nanoscale holographic interferometry for strain measurements in electronic devices. doi:10.1038/nature07049

In this manual, we will dive straight into the use of the sMoiré package with some worked examples. There is also a quick reference guide at the end of this document.

But before starting, there are a few important points to remember:

1. *sMoiré* is a *plug-in for DigitalMicrograph (Gatan)*. This means that results are fully compatible with the other functions present in DM. For example, the phase images produced, or strain maps, can be analysed or manipulated with functions like **Analysis...Statistics** or **Process...Simple Math**. However, if new images are produced by these operations, internal sMoiré variables will not be transferred.
2. *All the commands related to STEM Moiré Analysis* are located in the menu **sMoiré**:



3. The *only other additional feature* to DigitalMicrograph is located in the *Standard Tools Window*:

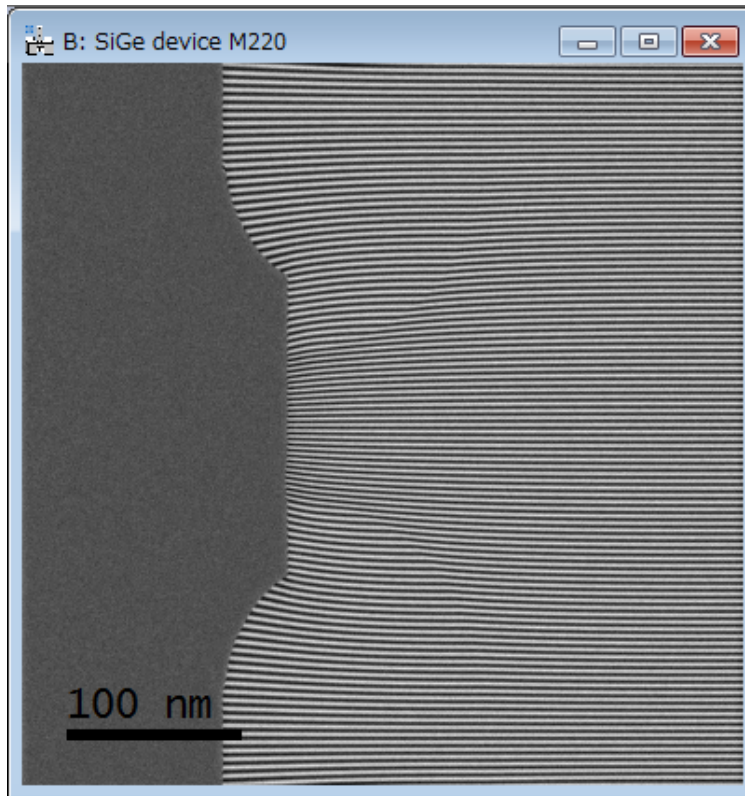


This **mouse tool** is a regular feature of other *HREM Research* plug-ins and is only used in sMoiré for the selection of spots in the *Power Spectrum*, as we will see.

# STEM Moiré Analysis Tutorial

## Getting Started

Open the STEM moiré image “SiGe device M220” using the DM command **File...Open** from the sMoiré Manual folder:



**Technical note:** this is an artificially constructed STEM moiré image. It represents a strained-silicon device with a realistic strain distribution.

**Important:** the image must be calibrated in nm/pixel. If not, use the DM **Analysis... Calibrate Tool** or magnification lookup tables.

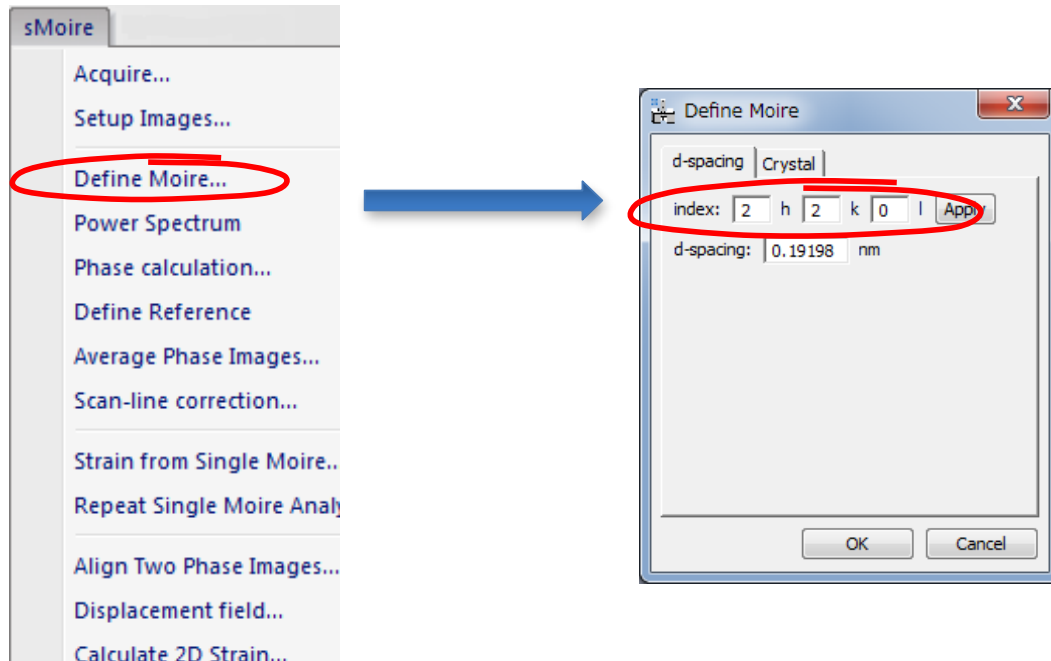
The example we have chosen has become a model system for strain mapping: a strained-silicon transistor with embedded SiGe sources and drains. Such devices have been studied by Geometric Phase Analysis (GPA Plug-in), Dark-field Electron Holography (HoloDark Plug-in), Nano-beam electron diffraction and more recently STEM moiré analysis. The SiGe sources and drains have a larger lattice parameter than the Si channel region and substrate and have been engineered to compress the Si in the channel under the gate.

This first example is a STEM moiré image made from the interference of the vertical scan with the (220) lattice planes. Finite element modelling has been used to create a realistic strain field.

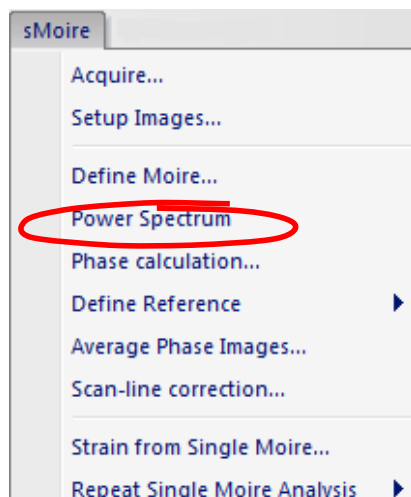
In this and the following examples, we assume that the microscopist carrying out the experiments (which may or may not be you!) has supplied the necessary information, notably:

- the lattice planes (index) close to the scan step,
- the approximate magnification of the image.

Firstly, you need to verify that the image has been calibrated, in our case indicated by the presence of a scale marker. Now you are ready to start STEM moiré analysis. At first you have to specify the lattice plane that will provides the moiré image. In order specify the lattice plane distance (d-spacing) you can use the index of the lattice plane and the crystallographic information (see details in the section Crystallography and Moiré definition).

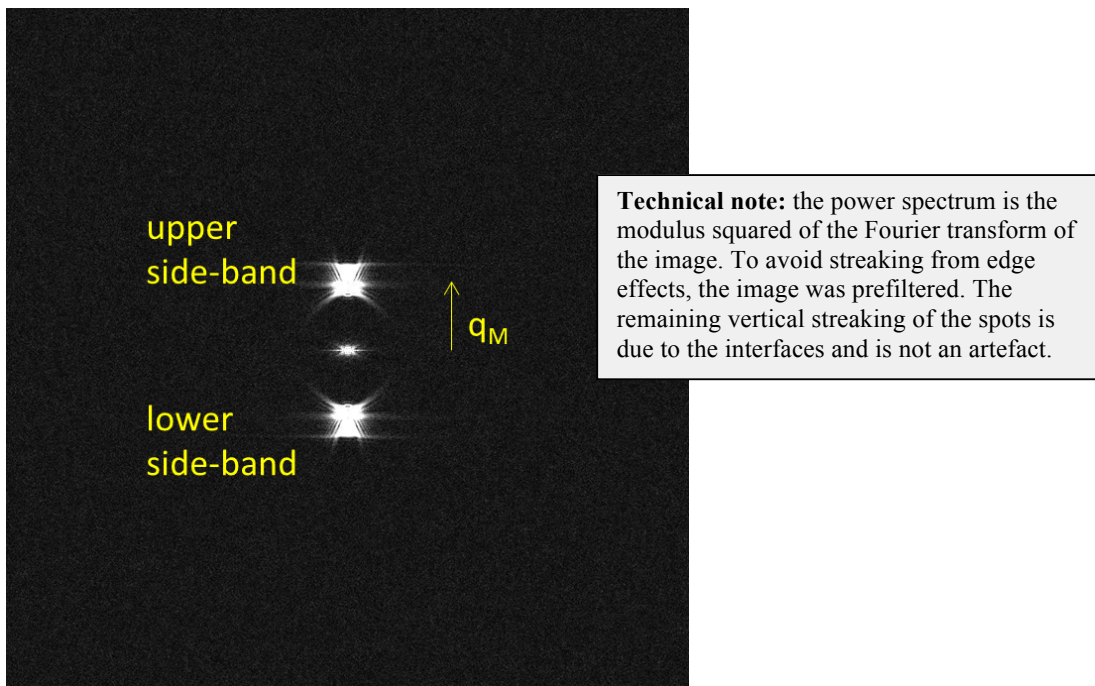


Next, you have to calculate the *Power Spectrum* of the image:




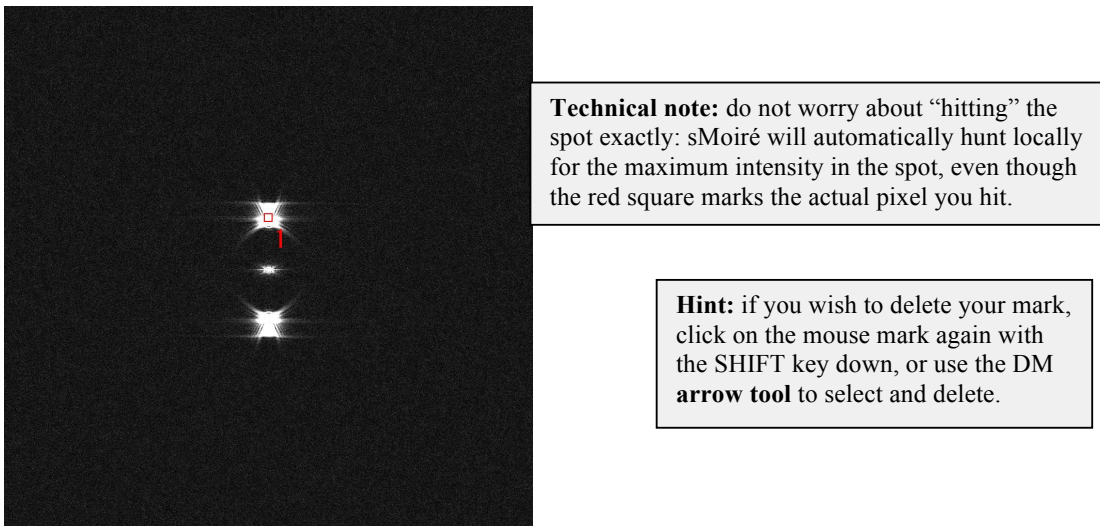
**Technical note:** in sMoiré, the STEM image does not have to be a power of two in size (e.g. 512 by 512).

You will see an image similar to this (without the annotation):



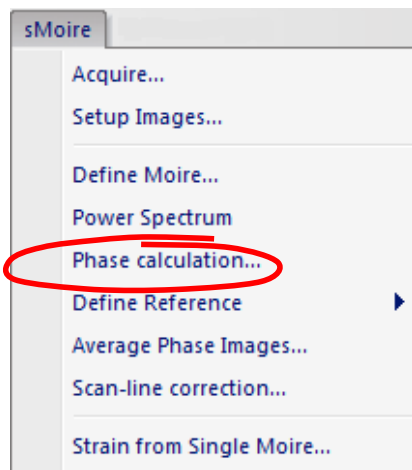
The Fourier transform consists of two “side bands” which contain the information on the moiré fringes, and hence the strain. We call the reciprocal vector which corresponds to the side-band frequency the “moiré frequency”,  $q_M$ . The moiré fringes will have a corresponding spacing,  $d_M$ , equal to  $1/q_M$ .

Now choose the **mouse tool**,  and click on the upper side-band towards the top. We will discuss later the choice of side-band.

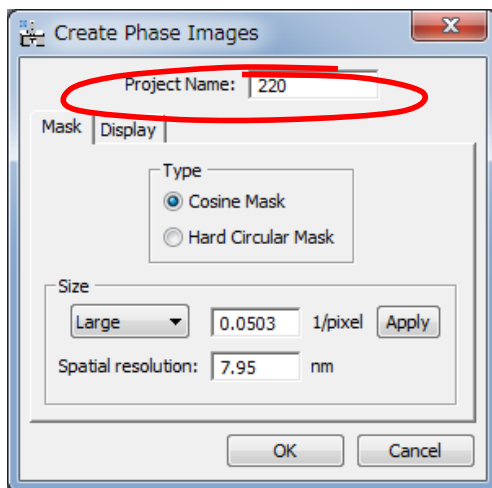




We are now ready to calculate our first *Phase Image* from the moiré fringes:

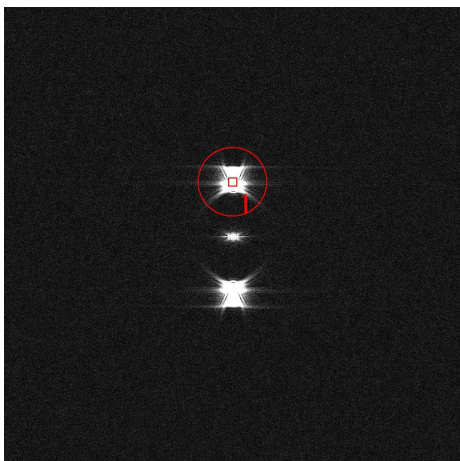


The following dialogue box will appear:



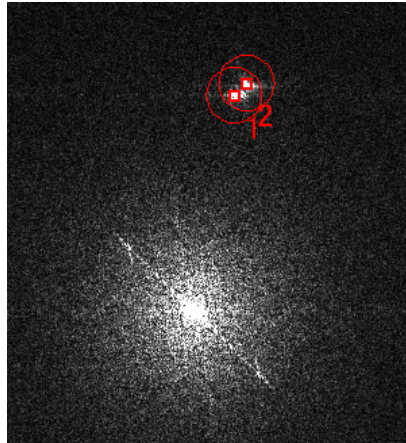
**Technical note:** in general we recommend the *Cosine Mask*. The *Square Mask* has been included as an option. The most important parameter is the mask size which determines the spatial resolution of the results.

The first choice, “Project Name”, gives the title prefix for all subsequent results e.g. phase images, strain maps etc. Choose a short name preferably and include the (hkl) indices of the lattice planes. For the mask type, use the default value of *Cosine Mask* for the moment. The most important parameter is the mask size (radius) and can be modified using the menu “Size” from Small (radius =  $q_M/4$ ), Medium ( $q_M/3$ ) to Large ( $q_M/2$ ). As you do this, the result of your choice will be seen on the *Power Spectrum*:



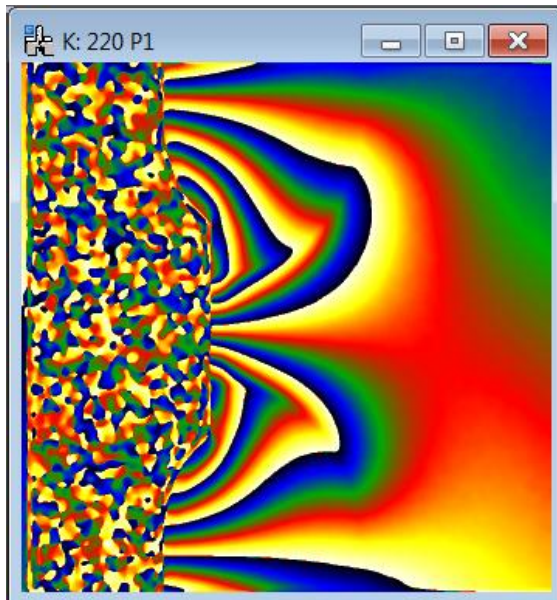
**Technical note:** the radius of the mask shows the area selected in Fourier space around the spot of interest. Decreasing the mask radius will produce smoother results but with less spatial resolution.

The maximum recommended size is  $q_M/2$  corresponding to the large mask size – the default value – and corresponds to a spatial resolution of  $2d_M$ , or twice the moiré fringe spacing.



**Tips:** In the STEM Moiré the difference of a lattice spacing or orientation between an interest area and the reference area is amplified by moiré effect. The right figure shows the case where the orientation change between two domains is only 0.3 degree, while we see a clear split of the spots. In such a case we can place more than one mask, and create a merge mask. Here, the first mouse point will be used as an initial estimate of the reference g-vector.

Now say OK and the phase image will appear:



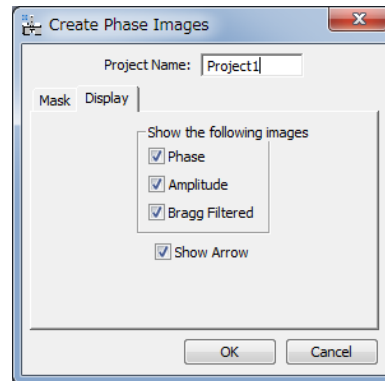
**Technical note:** sMoiré uses the “temperature” colour scale for displaying image values. If you prefer grey scales use the DM menu **Disaply... Image Display...Color**. Similarly, if you wish to change the maximum and minimum display values use DM menu **Object...Image Display...Contrast** or select an area on the histogram. In any case, the actual values in the image will not be changed, only its appearance.

This is the geometric phase corresponding to the moiré fringes and is proportional to the lateral shift of the fringes with respect to a perfect lattice. This is the image we will use to calculate the strain.

You should also see the amplitude image:

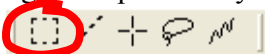


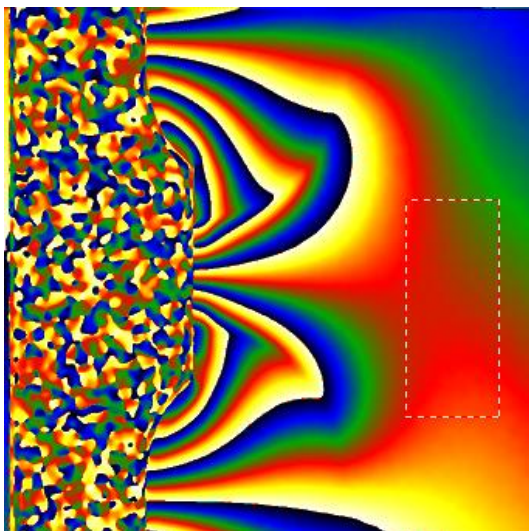
**Hint:** if you don't see this image, recalculate the phase image with **Phase Calculation...** and tick the "amplitude" box in the Display tab shown below.



The amplitude image corresponds to the local amplitude of the moiré fringes. For example, the black region corresponds to the area where there are no moiré fringes (see the original moiré image). We can see the layout of the specimen better in the amplitude and will be very useful later to align the phase images. If you check "Bragg filtered" box you will also get the image, where the moiré fringes are filtered out. The Bragg filtered image will be also useful later to align the images.

With the **Show Arrow** box ticked in the Display tab, you should see an arrow on the STEM Moiré image when you launch the Phase calculation command. (see Crystallography and Moiré definition)

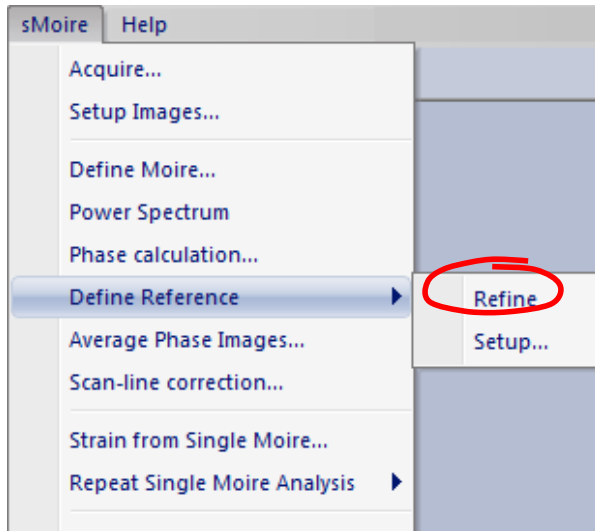
The next step is to define area which will correspond to a region of perfect crystal, e.g. in the substrate. Use the DM **ROI tool** (region of interest tool)  to select an area:



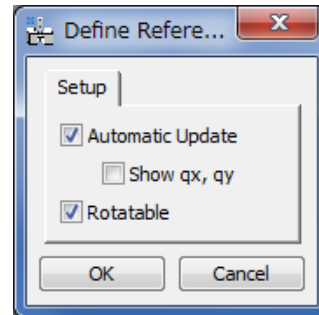
**Hint:** choose an area of smoothly varying phase (ideally uniform or of uniform gradient). Choose a reasonably big area for a better definition of the reference. Do not choose an area which straddles an interface.

It does not matter too much at this stage: you can move it as well as change its size later.

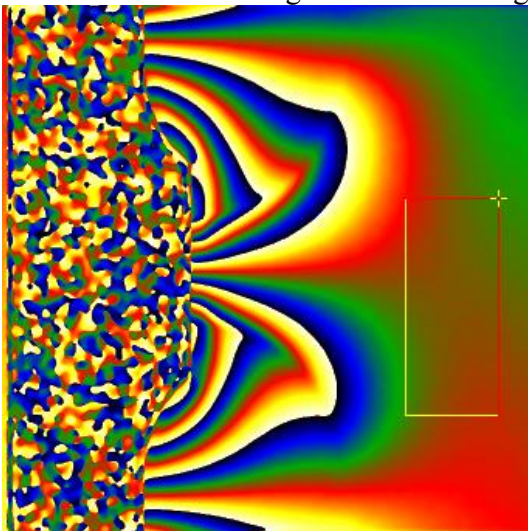
and then choose the next sMoiré command **Define Reference**.



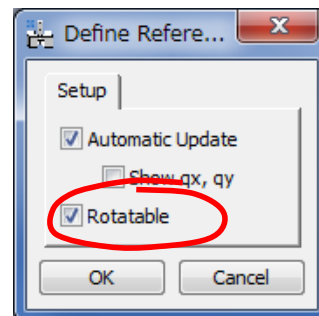
**Hint:** as mentioned above, if you do not like the reference area, just grab and slide the ROI across the image. sMoiré will automatically update the reference area. This function can be deactivated in **Define Reference...Setup**.



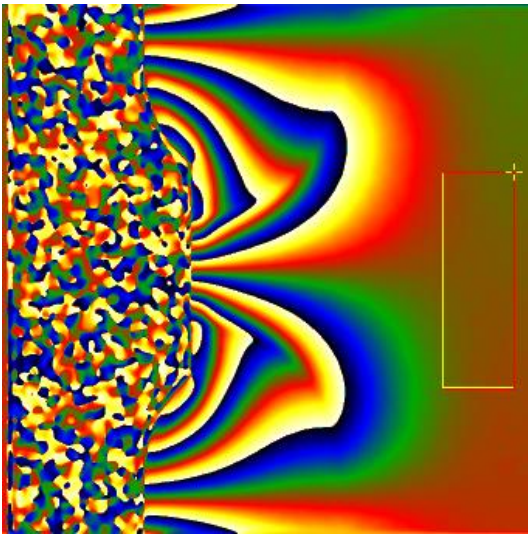
The result will be something like the following:



**Hint:** you can make this ROI rotatable by activating this feature in the **Define Reference...Setup**.



Adjust the shape and position of the ROI until the phase is nicely uniform within the ROI:



The phase image now has a well defined reference lattice. Do not worry about the “phase jumps” i.e. where the phase suddenly goes from black to white. This is quite normal and results from the normalisation of the phase between  $-\pi$  and  $\pi$ . Imagine the phase going round a circle anti-clockwise from 0 to  $\pi$  to  $-\pi$  (jump by  $-2\pi$ ) and back again 0. No discontinuity is present in the underlying moiré fringes.

The uniform area of phase shows the substrate (here in a brownish colour). The strained regions show up as regions of varying phase. The local gradient of the phase will determine the difference in lattice parameter and crystal orientation compared with the substrate.

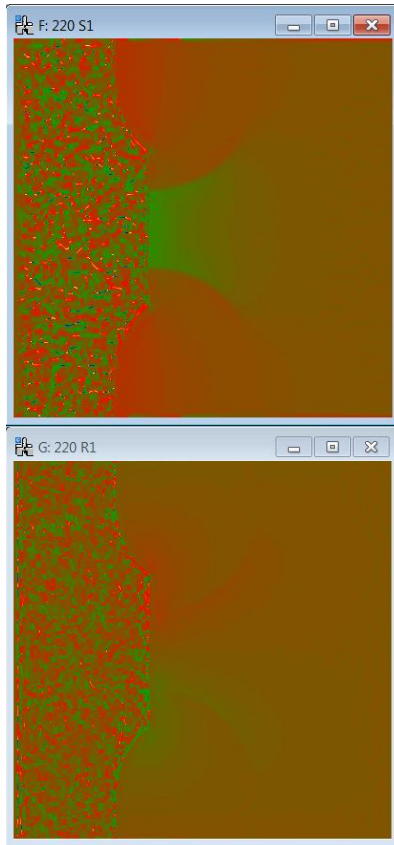
Here is the recommendation for the choice of reference area:

Choose an area with **known lattice parameter**  
which produces **uniform phase** after refinement  
and the **bigger the better**.



## Strain field

We can now determine the strain corresponding to these lattice planes. Use the sMoiré command **Strain from single moiré** and the following results will appear:

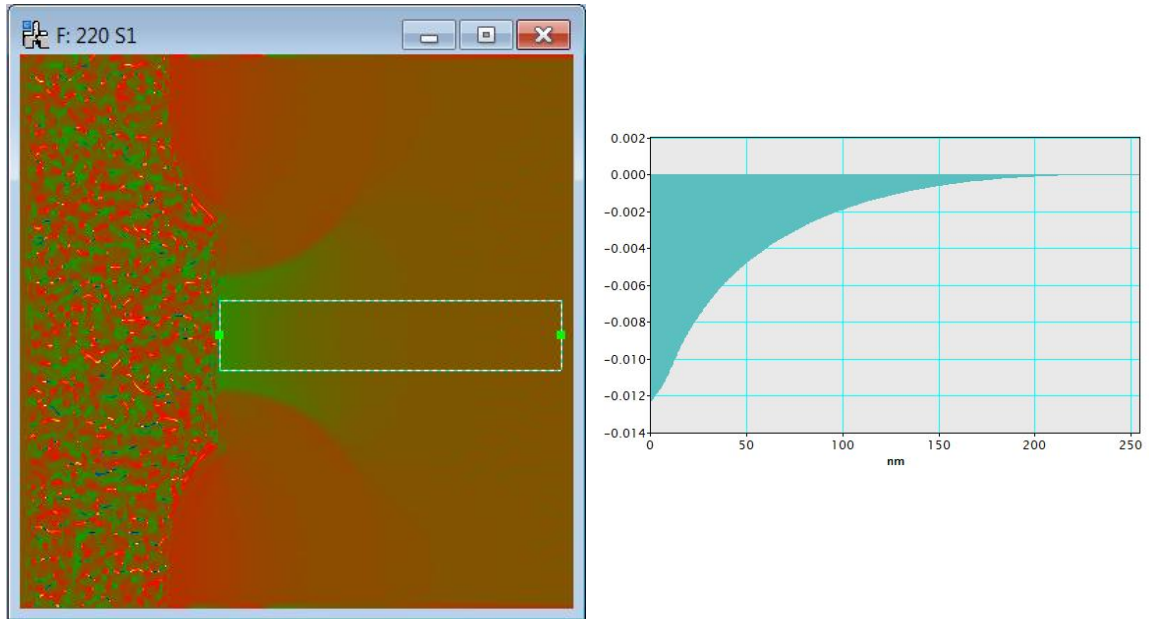


**Hint:** the colour scale has been chosen to be between -0.1 and +0.1 so that positive strain is a red or yellow colour and negative strains (compression) a green, or blue. The reference area should show up a brownish colour, equivalent to 0.

**Hint:** for rotations, the colour scale has been chosen by default to be between  $-10^\circ$  and  $+10^\circ$ . You can change these values as usual with the DM command **Display...Image Info...Contrast**.

The strain map, denoted S1 in the title, gives the change of the local lattice spacing with respect to the reference. A value of 0.05 means that the local lattice spacing is 5% bigger than the reference lattice. The red areas correspond to the SiGe sources and drains where the lattice is as much as 0.8% larger than the Si substrate. The green area is the channel region where the silicon is in compression. The rotation map, denoted R1 in the title, gives the in-plane rotation (in degrees) of the lattice planes.

These maps are fully quantitative and you can use all the DM tools to examine the strain. Below is an example using the Profile tool:



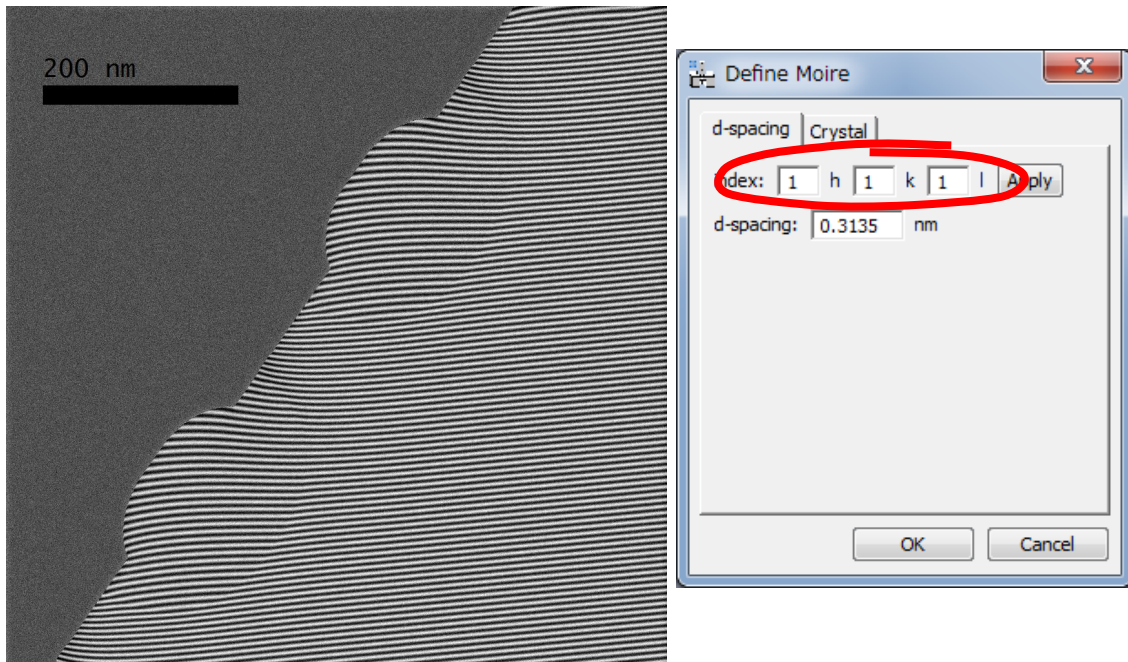
We can see that the strain reaches a value of -1.2% just under the gate.

To test these conclusions repeat the full analysis on the image “SiGe device M200 – angle”. This moiré image simulates the case where the vertical scan is not exactly parallel to the [220] direction. You will see that the moiré fringes are rotated but that the strain measured is identical to the previous case.

This is where many applications of **strain mapping** end with a strain component measured in one direction. However **sMoiré** allows for more sophisticated analysis and the determination of the **full 2D strain tensor** as the next section explains.

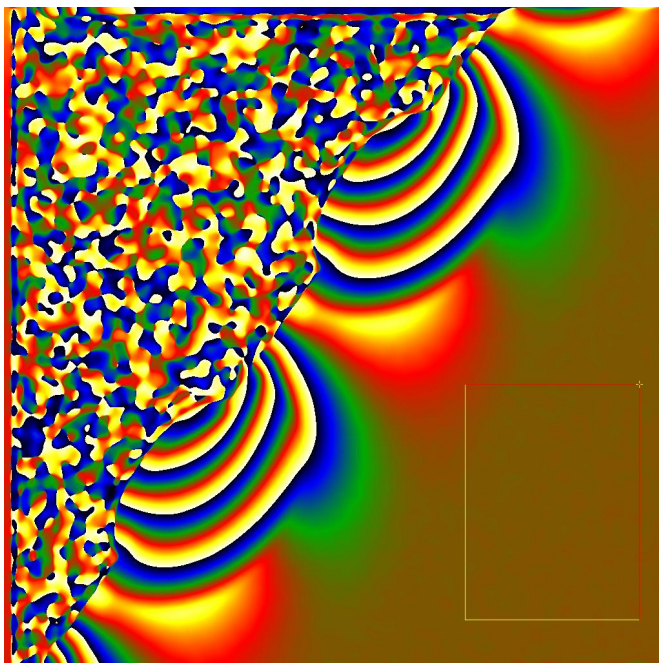
## Determining 2D strain tensors

In order to measure a 2D strain tensor, moiré fringes need to be created for two non-parallel lattice planes. Open the image “SiGe device M111”:



The vertical scan direction has been chosen to be parallel to the  $[111]$  direction, with a scan step slightly bigger than twice the  $d_{111}$  spacing. Initial calibration gives 0.66 nm per pixel.

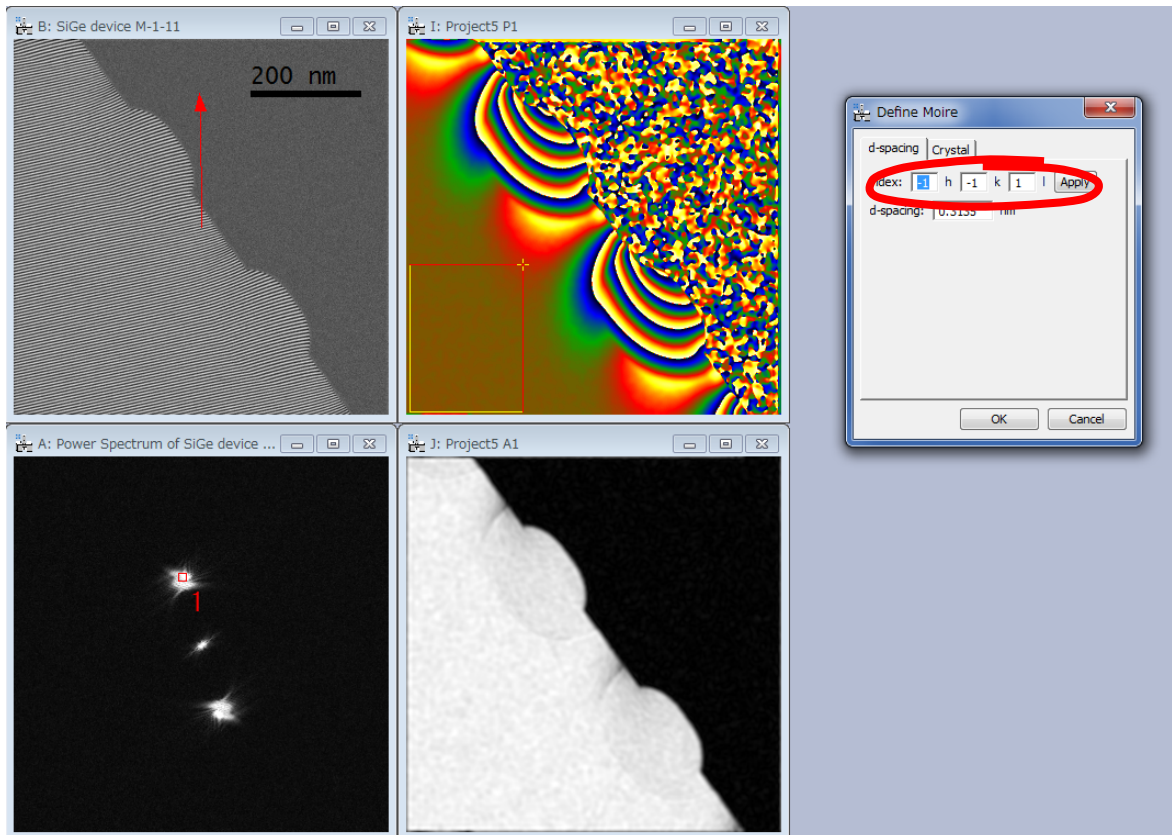
Calculate the phase image and define a suitable reference region as for the previous section:



You might like to rotate the reference region, as shown above, and make sure you also calculate the amplitude image that will be necessary for the alignment step later.



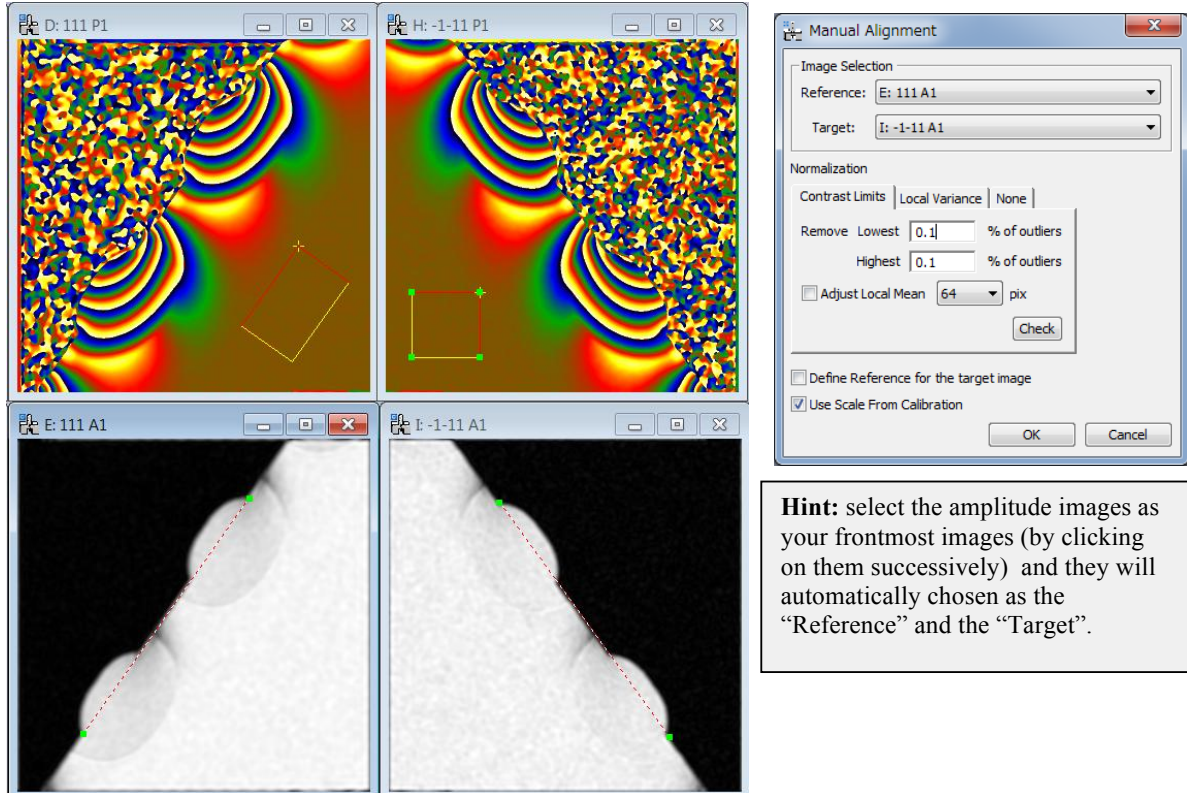
Repeat the analysis for the other moiré image created from the (-1-11) lattice planes “SiGe device -1-11”:



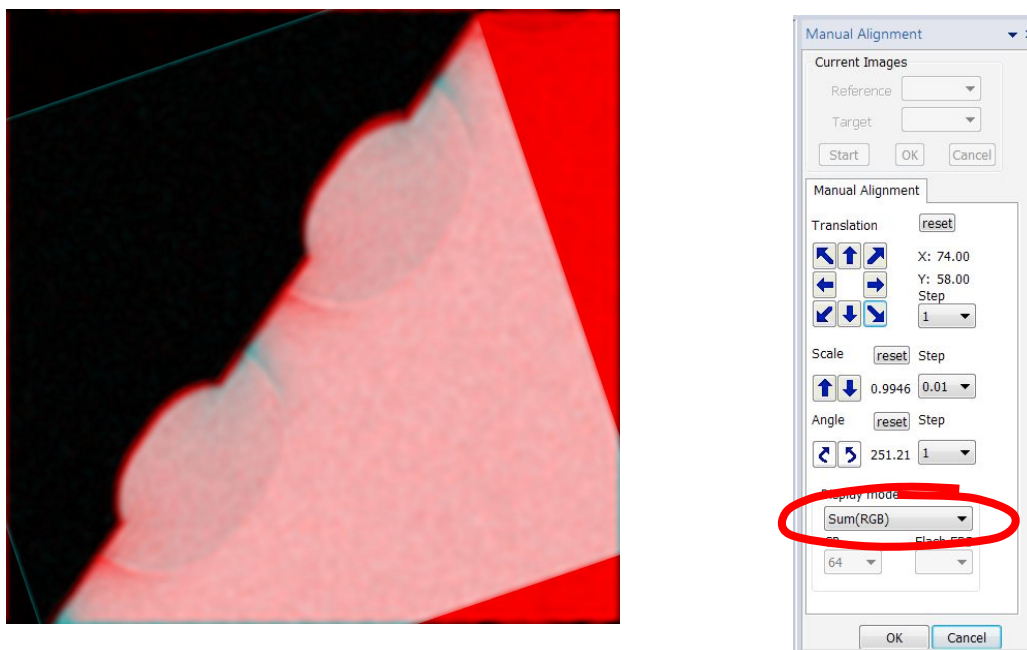
For cubic silicon, you do not actually need to provide the exact indexing of the lattice planes, just the family name important for the d-spacing. We have also been increasingly sloppy in the orientation of the scan with respect to the lattice planes and even the magnification has changed slightly with respect to the (111) moiré image. This is to show that **sMoiré** is capable of handling such experimental vagaries.

## Image alignment

The two moiré images are necessarily rotated with respect to each other, so the phase images need to be aligned before calculating the strain field. Place the images next to each other and use the **DM Line ROI tool** to indicate identical areas on the two amplitude images:

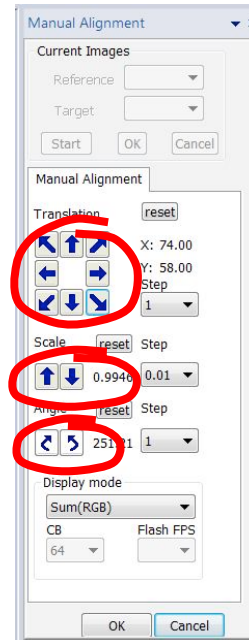
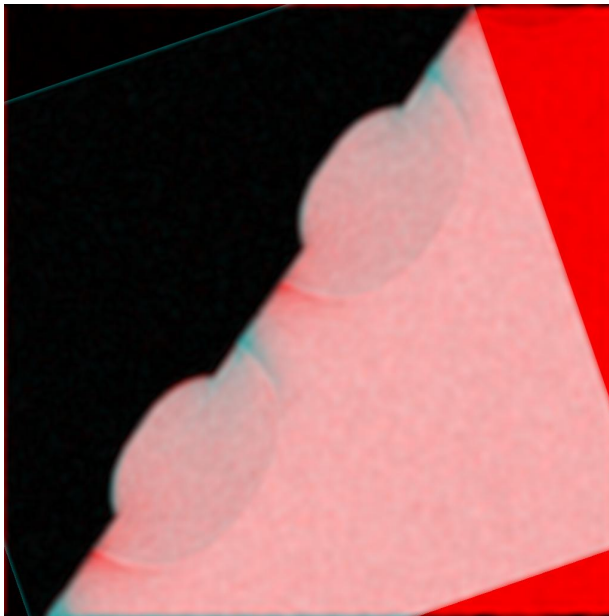


Launch the sMoiré command **Align Two Phase Images...** using the default settings and the following image and window should appear:

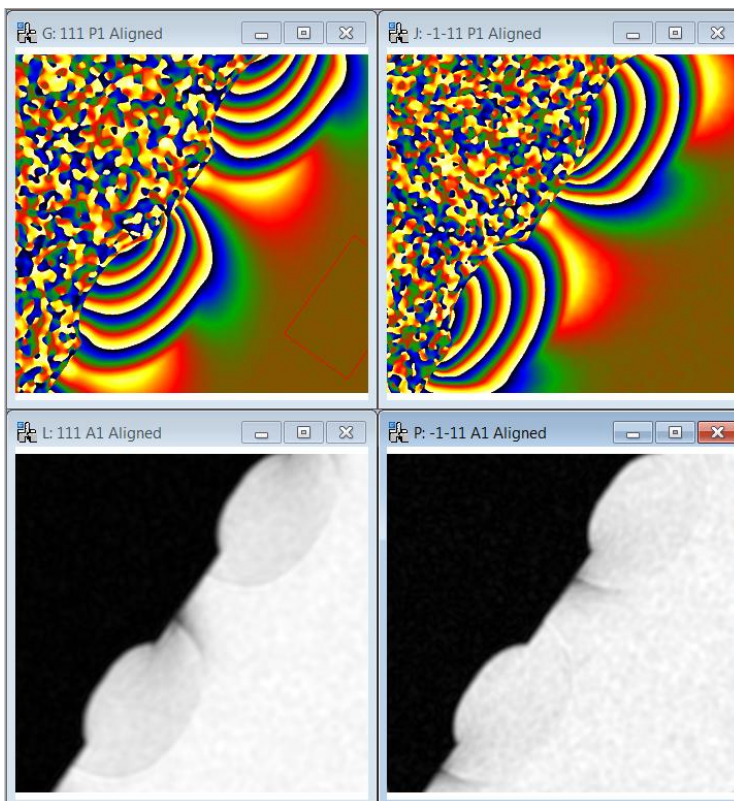


If it does not look anything like this, you may need to check that you chose the 111 amplitude as the “Reference” and the -1-11 amplitude as the “Target”, or that you have placed the Line ROI correctly.

Using the Display mode “Sum(RBG)” the two images are overlaid with red and green areas indicating unmatched areas.



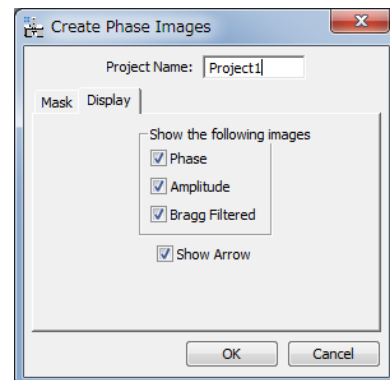
Use the different functions of Translation, Scale and Angle to align the two images the best you can. The result will never be perfect as the two images will always be slightly different in contrast. The best guides are sharp edges, like the surface of the sample here. Once you are happy, press on the OK button.



The program has used the alignment of the amplitude images to align the phase images. The images have been cropped to have all the same size. Now it is possible to calculate the strain field.

**Technical note:** Here, we have used the Amplitude images to align two moiré images. You can also use Bragg Filtered images to align the moiré images. The Bragg filtered image will filter out the moiré fringes, and is close to the center-band image, while the Amplitude image is a side-band image. In the real experimental moiré images the Bragg Filtered images often work better than the Amplitude images. You can try two filtered images for your experimental moiré images.

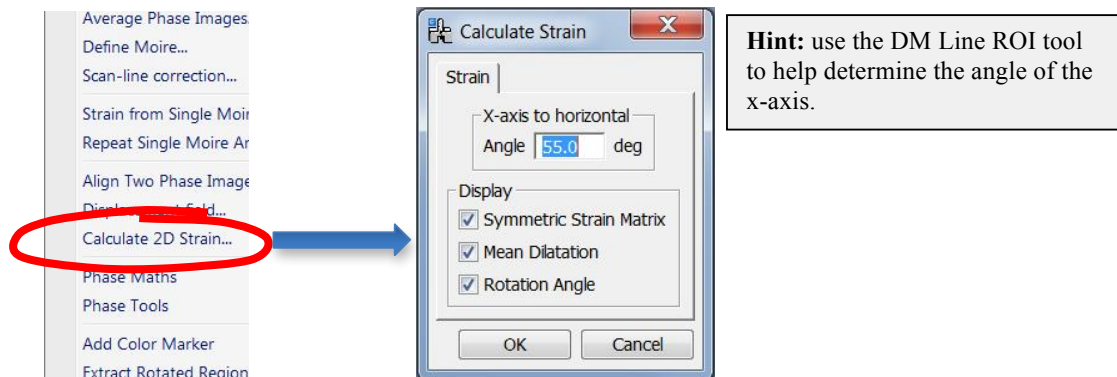
**Hint:** if you don't see the Bragg filtered image, recalculate the phase image with **Phase Calculation...** and tick the "Bragg Filtered" box in the Display tab shown below.



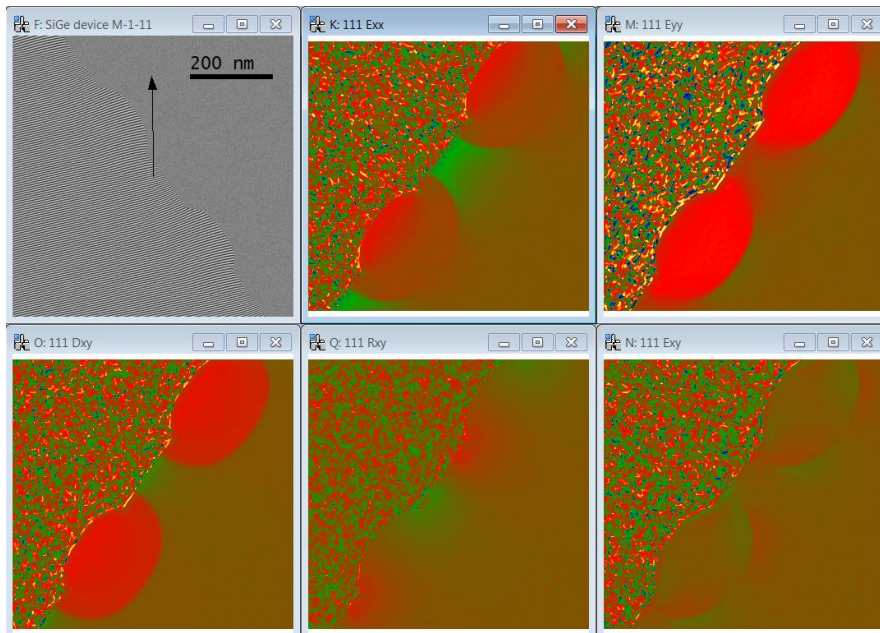


## 2D strain field

Select the two aligned phase images and launch the sMoiré command **Calculate 2D Strain...**

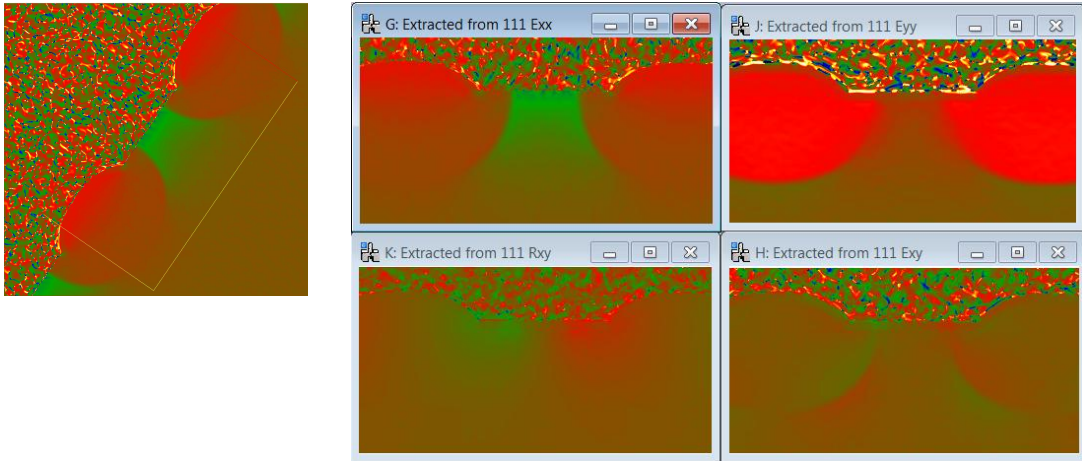


Choose the x-axis to be parallel to the surface of the sample, and hence the y-axis in the growth direction.



In addition to the  $E_{xx}$  component, which was actually determined in the previous example, the other strain components are revealed:  $E_{yy}$  the strain in the growth direction,  $D_{xy}$  the dilatation or average of  $E_{xx}$  and  $E_{yy}$ ,  $E_{xy}$  the shear, and  $R_{xy}$  the in-plane rigid-body rotation (in degrees).

For the final flourish, place a DM rectangular ROI on one of the strain maps, say  $E_{xx}$ , and use the sMoiré command **Extract Rotated Region...Define** to make the rectangular ROI rotatable. Then, rotate and adjust the shape and size of the rotatable ROI. Now use **Extract Rotated Region...Extract group** and a number of windows will appear:

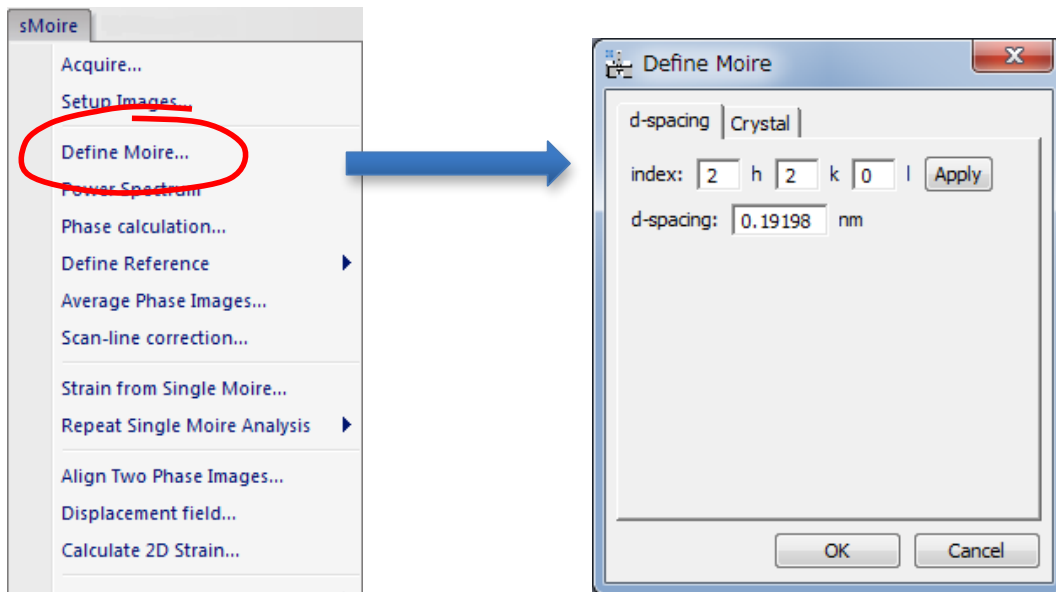


Add a scale marker with **DM Edit...Data Bar...Add Scale Marker** and finally sMoiré command **Add Color Marker** and the results are nearly ready to publish!

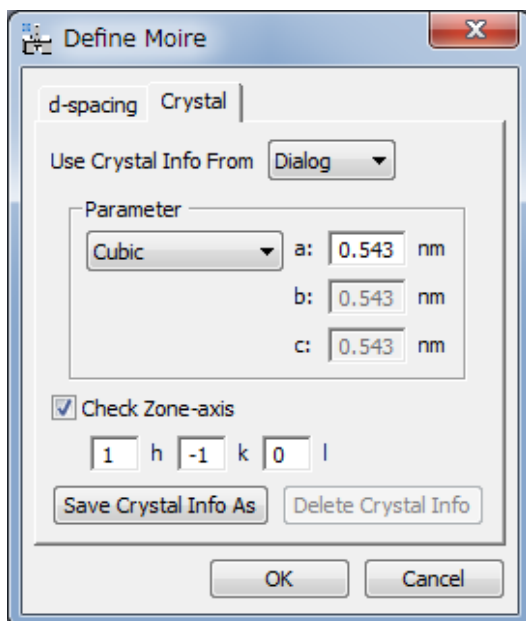
This marks the end of the tutorial. Now it is time to enjoy analyzing your own data with **STEM Moiré Analysis**.

## Crystallography and Moiré definition

STEM Moiré Analysis requires knowledge of the specimen crystallography and orientation (notably zone-axis) in order to interpret the moiré fringes. To enter these, use the sMoiré command **Define Moiré...**:



Before filling in the details in the **d-spacing** tab, you need to input the crystal structure in the **Crystal** tab.

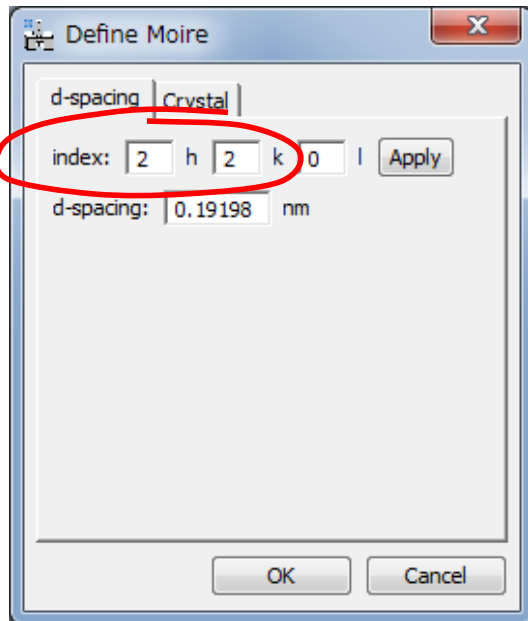


**Technical note:** for the moment sMoiré can only deal with cubic, tetragonal and orthorhombic crystals.

**Technical note:** The zone-axis information is optional. The program will warn you if the d-spacing index is not perpendicular to the zone axis.

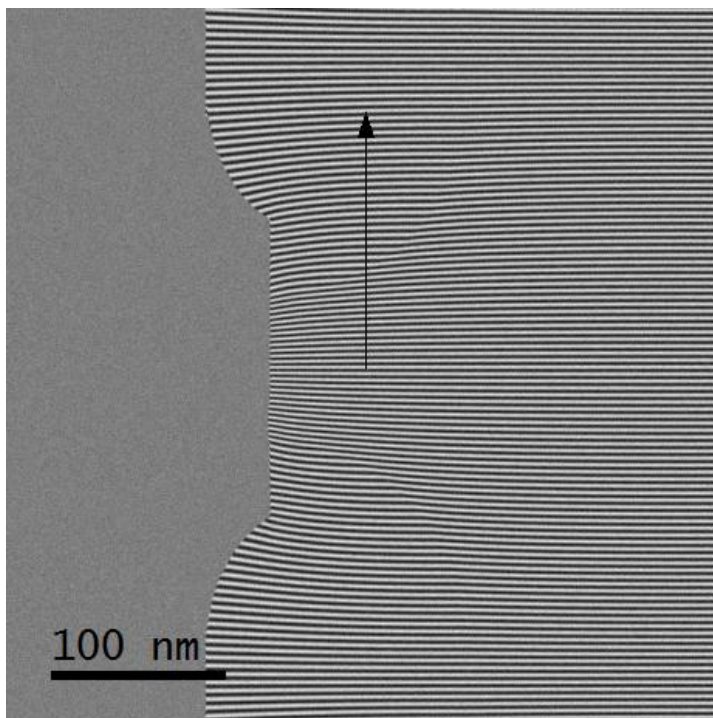
The example is Silicon, which is cubic with a lattice parameter of 0.543 nm, as shown. The zone-axis is [1-10]. If “Use Crystal Info from” is “Dialog,” the crystal setting currently shown in the dialog will be used. You can save/delete the crystal setting and use it later.

You now need to tell sMoiré the lattice planes that create the moiré contrast. This can be done using the **d-spacing** tab:



**Hint:** if you change the indexes, you need to press on the **Apply** button to update the “d-spacing”.

You need to indicate the lattice planes which lie horizontally i.e. with a g-vector that creates the moirés in the direction of the vertical scan. In this case the (220) lattice planes are indicated. With the **Show Arrow** ticked in the Display tab of the Phase calculation dialog, you should see an arrow appearing on the STEM Moiré image:



There is more to **Define moiré...** than meets the eye. The program has compared the (220) lattice spacing with the vertical scan step, which can be multiples of the lattice spacing. The program has then determined the exact direction of the (220) reciprocal lattice vector, which is not necessarily parallel to the scan. The arrow indicates this exact direction of the g-vector on the original moiré image.

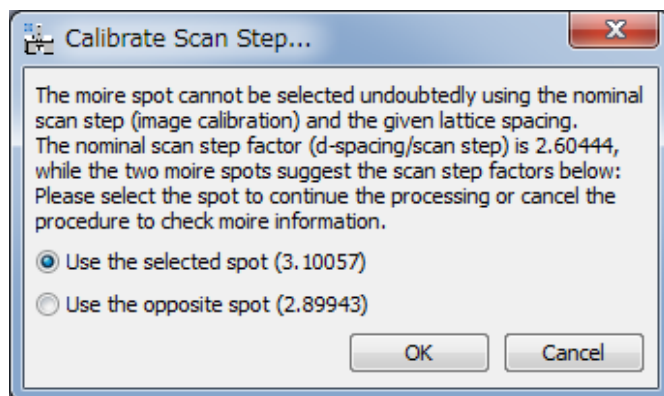


Knowing the lattice spacing, the moiré fringe orientation and spacing, it can recalibrate the scan step exactly. Use the DM command **Display...Image Info...Calibration** to see that the original moiré image was calibrated at 0.4 nm per pixel, whereas the calibration of the phase image is now 0.403175 nm per pixel. This function will work correctly provided that the initial calibration was good enough to indicate that the scan step was either bigger, or smaller, than the lattice spacing, or indeed multiples of the lattice spacing. Let us examine this example more carefully to see what this means.

In the sample moiré image the lattice planes creating the moiré effect have a spacing of  $d_{220} = 0.1920$  nm, and the moiré spot is located at  $q_M = 0.1$  pixel<sup>-1</sup>. Since the original moiré image was *nominally* calibrated at 0.4 nm per pixel, the *true* scan step is close to the image calibration. The *nominal* scan step factor  $s_F$  is given for the *nominal* calibrating as (scan step)/(lattice spacing) = 0.4 nm/0.1920 nm = 2.08. Thus, the scan step should be close to twice the  $d_{220}$ , and the *true* scan step factor is  $2 + q_M = 2.10$ . Therefore, the *true* scan step should be 0.4032 nm (2.10 x 0.1920 nm).

What happen if we choose the opposite moiré spot, when calculating the phase image? The program chooses automatically a correct moiré spot, and calculates the correct scan step as 0.4032 nm. Thus, you can choose either moiré spot, if you know a sufficiently accurate scan step, namely the moiré image is calibrated with sufficient accuracy.

If the program cannot choose the right moiré spot and determine the true scan step using the given calibration (the scan step), the following window will appear when you calculate the phase image:



If you get this message, it is better to check the nominal calibration or the lattice plane index. If you select the opposite spot, the mouse point appears at the opposite moiré spot on the original moiré image.

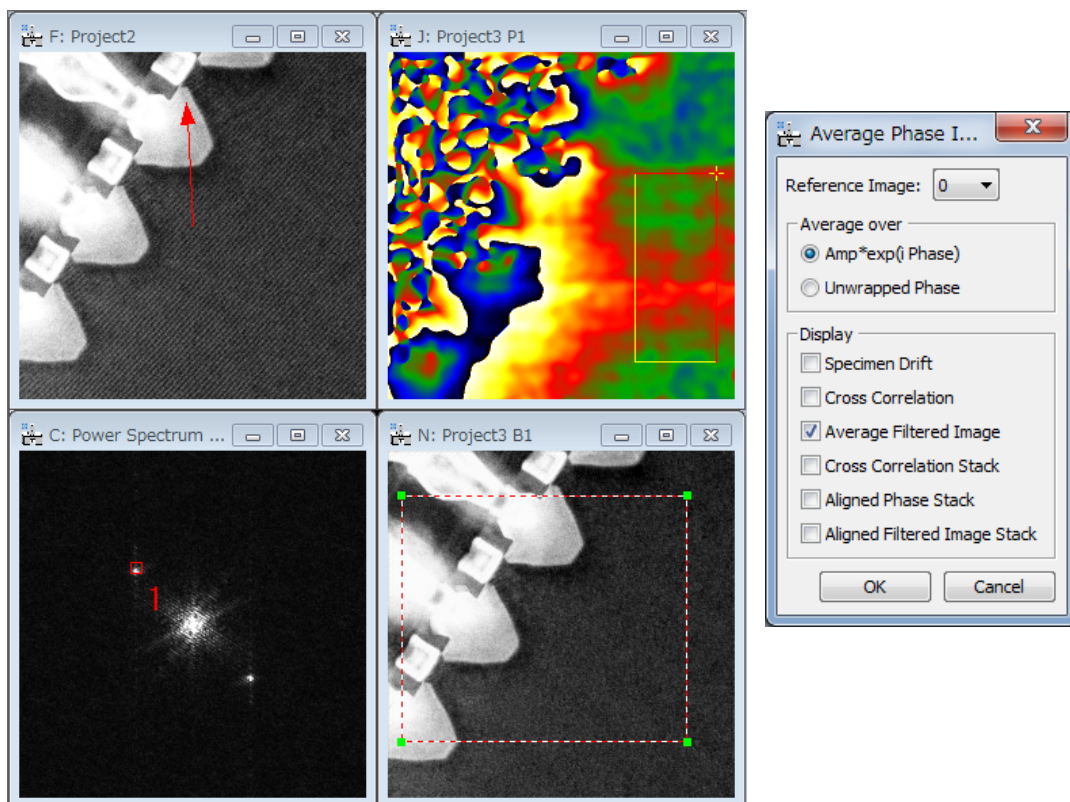
**Technical note:** The sMoiré program can handle the moiré pattern created by the sampling interval that is close to a multiple of the lattice spacing. Here, we assume the moiré spot is located at  $q_M$  pixel<sup>-1</sup>. If the scan step  $s$  is close to the lattice spacing of  $d$ , the inverse of the scan step ( $s^* = 1/s$ ) will be close to the g-vector ( $d^* = 1/d$ ) (namely,  $s^* \approx d^*$ ), and thus  $d^* = (1 \pm q_M) \times s^*$ . However, if the scan step is close to  $n$ -times of the  $d$  spacing, the inverse of the scan step will be close to the  $d^*/n$ , and thus  $d^* = (n \pm q_M) \times s^*$ . Thus,  $s = (n \pm q_M) \times d$  for the sampling step is close to  $n$ -times of the spacing. Here, we define the scan step factor  $s_F = (\text{scan step})/(\text{lattice spacing}) = n \pm q_M$ . Then, the *true* scan step (the *accurate* image calibration) is calculated as  $s_F \times (\text{lattice spacing})$ . Thus, we don't need to calibrate the scan step accurately, if we know the lattice spacing and an approximate scan step.

## STEM Moiré Image Series

The image quality is important for strain analysis. Thus, the sMoiré works for STEM moiré image stack as well as a single moiré image. If the front image is a stack of STEM moiré image, the selected command, say **Power Spectrum...** or **Phase calculation...**, perform its job automatically for each moiré image and gives a stack of the result images.

### Average Phase Images

This is a command specific to a STEM Moiré image stack. At first, place a *Rectangular ROI* on a filtered image stack, namely an amplitude image stack or a Bragg filtered image stack. Here, the Bragg filtered image stack B1 will be used as a reference image to determine the image drift. When you launch **Average Phase Images** command, the dialog shown below right will appear:

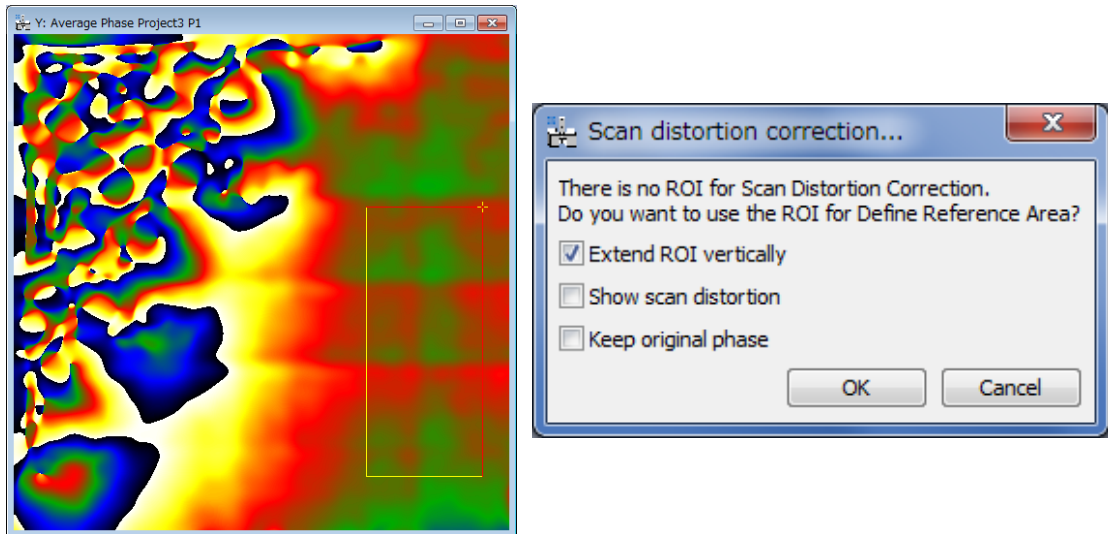


Here, you can choose how the phase images are averaged, namely over the complex amplitude ( $\text{Amp} \times \exp(i \text{Phase})$ ) of each moiré side-band image or the unwrapped phase of each image. You can also select the results to be displayed. Of course, the average phase image is always displayed.

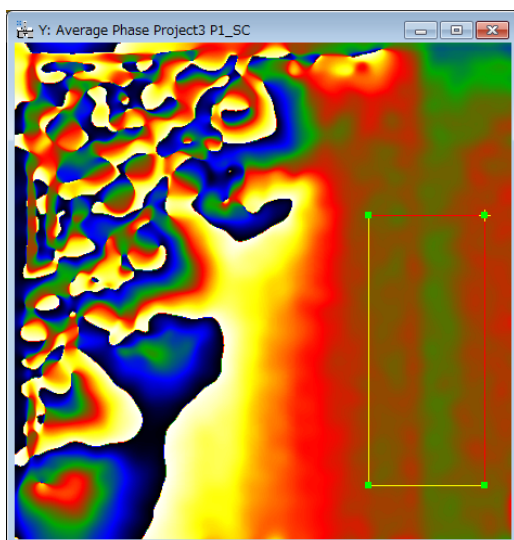
## Scan-line Correction

The scanning system is not always perfect, and the phase image often gives horizontal bands as shown below. If there is the region in the phase image, where you believe no distortion is expected, or the distortion will be small, we can correct the scan-line distortion using the geometrical phase analysis (GPA). Thus is because the *geometrical* phase image should be flat over the region with no distortion.

At first, place a *Rectangular ROI* on an averaged phase image, and then launch **Scan-line Correction** command. You will get the dialog shown below right:

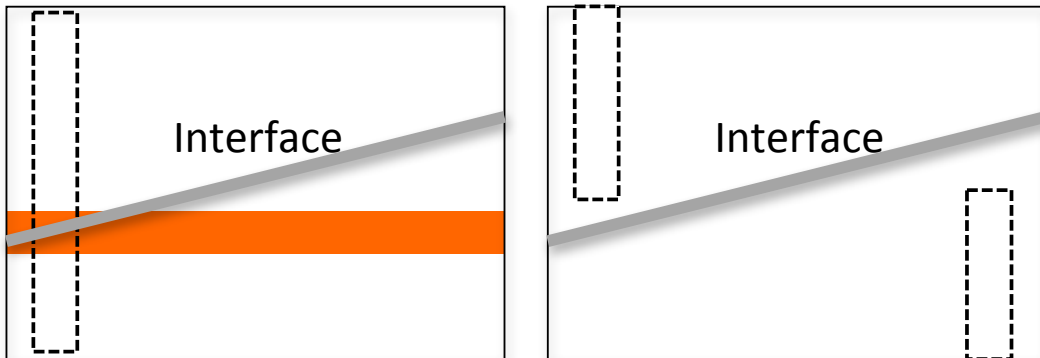


Here, the *Extend ROI vertically* option ensures that the distortion correction is carried out from top to bottom of the whole image. Then, you will get the scan-line corrected phase image as shown below:



The scan-line correction has a capability to merge multiple reference areas in the image. Here, we consider the case where there is an inclined interface across the image. If we define the reference area from top to bottom, the scan-line correction does not work where the reference

area intersects the interface as shown below left. In this case, we can use two reference areas at the top left and the bottom right as shown in below right. Then, the scan-line correction works better by combining scan-line information from these two reference areas.



## Appendixes

### A: Important phase relations

Strain tensor for small deformations:

$$\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \text{ i.e. } \varepsilon_{xx} = \frac{\partial u_x}{\partial x}, \varepsilon_{yy} = \frac{\partial u_y}{\partial y}, \varepsilon_{xy} = \frac{1}{2} \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right)$$

Mean dilatation :

$$\Delta_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_i} + \frac{\partial u_j}{\partial x_j} \right) \text{ i.e. } \Delta_{xy} = \frac{1}{2} (\varepsilon_{xx} + \varepsilon_{yy})$$

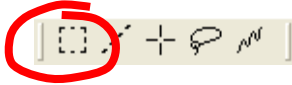
Rotation (in radians and anti-clockwise positive):

$$\omega_{ij} = \frac{1}{2} \left( \frac{\partial u_j}{\partial x_i} - \frac{\partial u_i}{\partial x_j} \right) \text{ i.e. } \omega_{xy} = \frac{1}{2} \left( \frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y} \right)$$

**Note:** these relations are only valid for small deformations. However, sMoiré uses the full relations suitable for large deformations (see Appendix in Hytch, Snoeck, Kilaas.)

## B: Useful DigitalMicrograph commands

DM ROI tool:



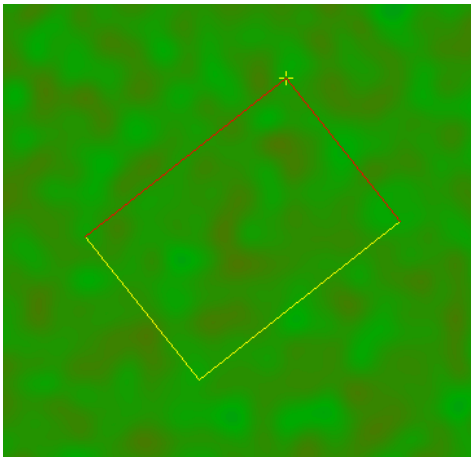
**Hint:** to select a square area, hold down SHIFT.  
To select powers of two, hold down SHIFT-ALT.

DM magnifying glass:



**Hint:** to demagnify, press ALT.

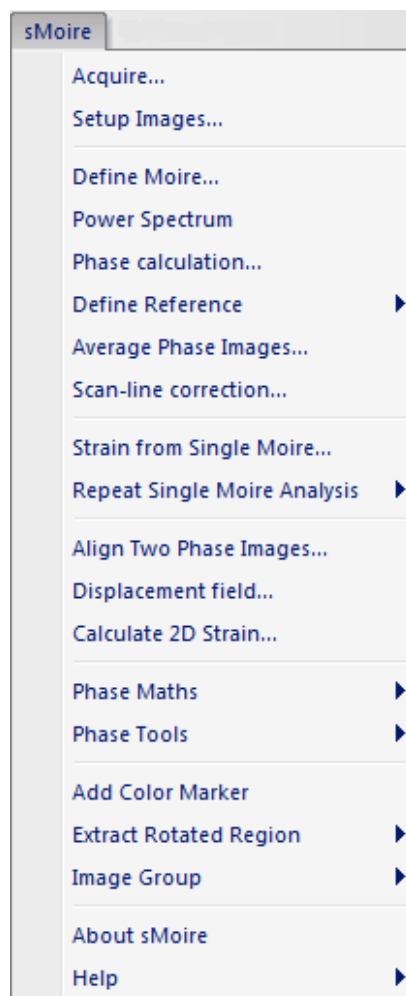
## C: Rotatable ROI



The edge length will be adjusted by one of the yellow edges, and the rotation angle will be adjusted by the yellow cross (+). (You can change the both edge lengths by dragging the yellow cross when pushing the SHIFT key.)

# Quick Reference Guide

## The sMoiré Main Menu



The commands in the sMoiré menu are described below.

Command	Description
Acquire...	Acquire a series of STEM Moiré images using the DigiScan under the current microscope conditions.
Setup Images...	Set up a stacked image from a set of saved individual images.
Define Moiré...	Specify the lattice plane that creates the STEM Moiré image.
Power Spectrum	Calculates and displays the Fourier transform of the front most STEM Moiré image. The centre of a Moiré spot is then selected in the Fourier transform (called Power Spectrum) using the mouse tool.

Phase calculation...	Calculates phase image for the Moiré spot selected in the Power Spectrum (see options).
Define Reference (see sub menus)	Menu concerning the reference region. You can use this command to refine the reference region simultaneously on two images after alignment.
Average Phase Images...	Calculates an average phase after registering the phase images using the corresponding filtered images (amplitude or Bragg filtered image).
Scan-line correction...	Corrects “fly-back” scan distortion in STEM using an average value measured within the user specified ROI.
Strain from Single Moiré...	Calculates strain component perpendicular to the lattice planes (i.e., parallel to the diffraction vector).
Repeat Single Moiré Analysis (see sub menus)	Repeats the same analysis as the most recent analysis or the previously saved analysis.
Align Two Phase Images...	Allows two phase images from different Moiré images to be aligned. Corresponding filtered images (amplitude or Bragg filtered image) will be used to find alignment conditions.
Displacement Field...	Calculates the full 2D vector displacements in the plane of the image from two phase images (see options).
Calculate 2D Strain...	Calculates the two-dimensional deformation tensor. Asks for two phase images and options (see below).
Phase Maths (see sub menus)	Menu of different mathematical operations which can be performed on phase images.
Phase Tools (see sub menus)	Menu of useful operations, not necessarily restricted to phase images.
Add Color Marker	Adds a color bar and the low and high display ranges. You can move the whole color marker or change its size. Since the display ranges are text annotations, you can move and edit them as you like. The color marker can be placed outside of the image display. You can rotate and flip using Edit commands. (The ratio of the color bar is fixed.)
Extract Rotated Region (see sub menus)	Extracts a region(s) of interest from the processed image(s). The region to be extracted can be arbitrarily rotated, and then the long edge direction will be rotated to horizontal.
Image Group (see sub menus)	Menu to close or save groups of images that are related with each other, e.g. strain maps.



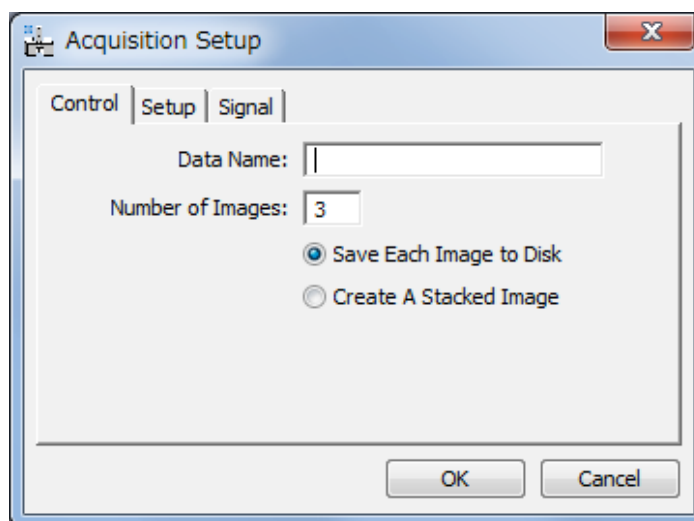
## Acquire Menu

### Acquisition Setup Dialog

The components of the dialog are described below.

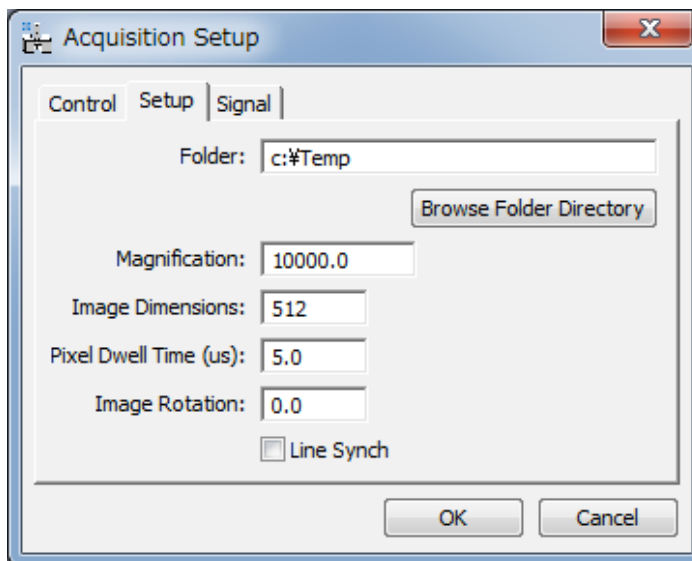
Component	Description
Control Tab	For information about the components of the Control tab, see <a href="#">Control Tab</a> below.
Setup Tab	For information about the components of the Setup tab, see <a href="#">Setup Tab</a> below.
Signal Tab	For information about the components of the Signal tab, see <a href="#">Signal Tab</a> below.
OK	Closes the dialog and acquires the specified number of images according to the specified parameters.
Cancel	Closes the dialog without executing the command.

#### Control Tab



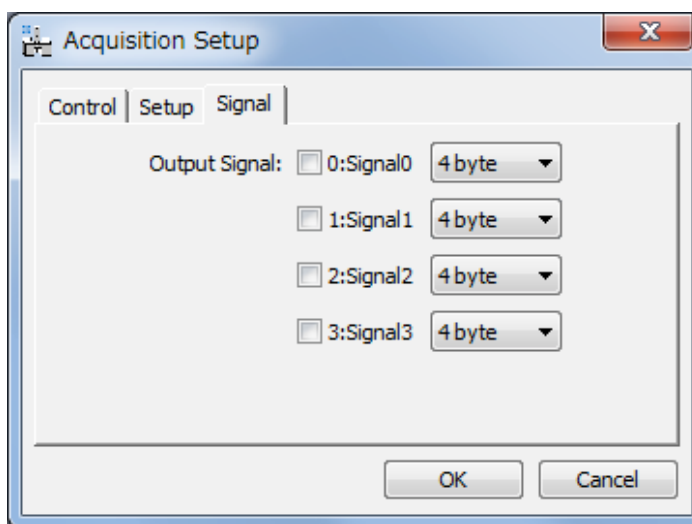
Component	Description
Data Name	Acquired images will be identified with this name and an added sequential number.
Number of Images	Acquired number of images (positive number).

**Setup Tab**



Component	Description
Folder	Acquired images will be saved into this folder, when 'Save Image to Disk' is selected. You can browse the folder directory.
Magnification	Image magnification (This will be read from your microscope, if possible.)
Image Dimensions	Image size (width and height in pixel).
Pixel Dwell Time	Pixel dwell time (in microseconds)
Image Rotation	Rotation angle of Acquired images.
Line Synch	If checked, a hardware line synch will be applied.

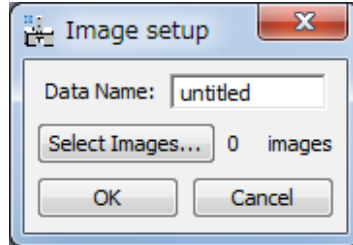
**Signal Tab**



Option	Description
Output Signal	Select signal and data length for each output signal.

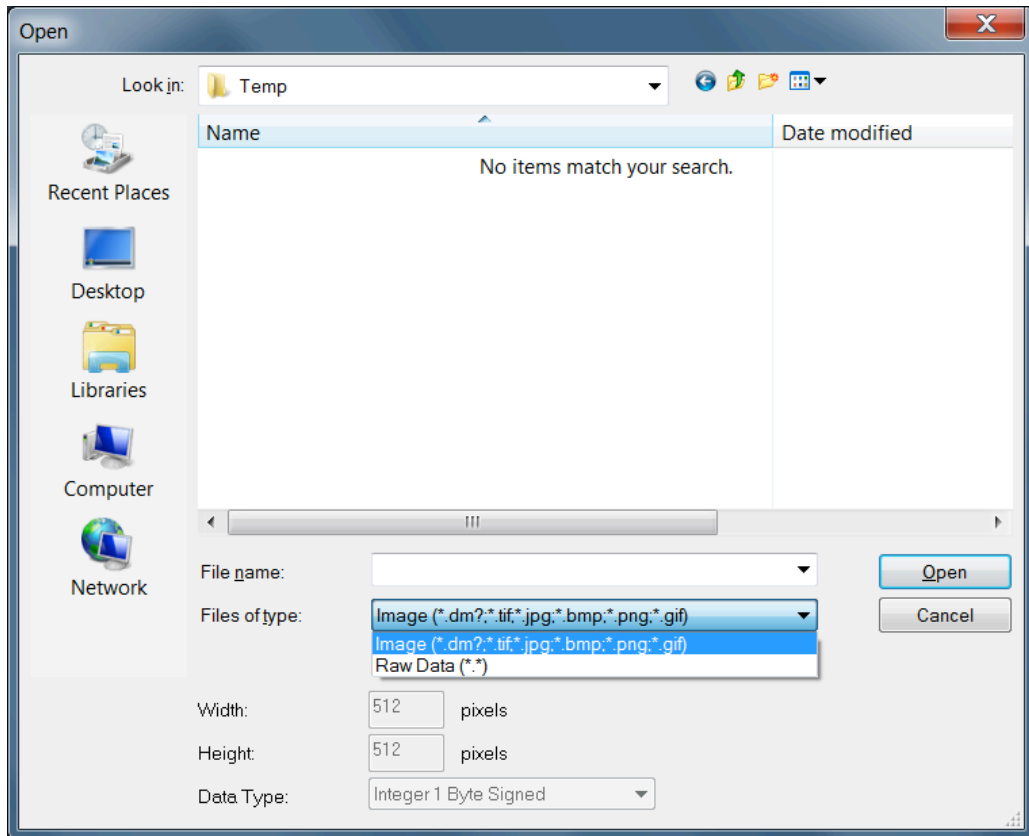
## Setup Images Menu

### Setup Images Dialog



Component	Description
Data Name	Specify an unique data name for the stacked image
Select Images...	Opens a File Open dialog to select archived images.

### File Open Dialog

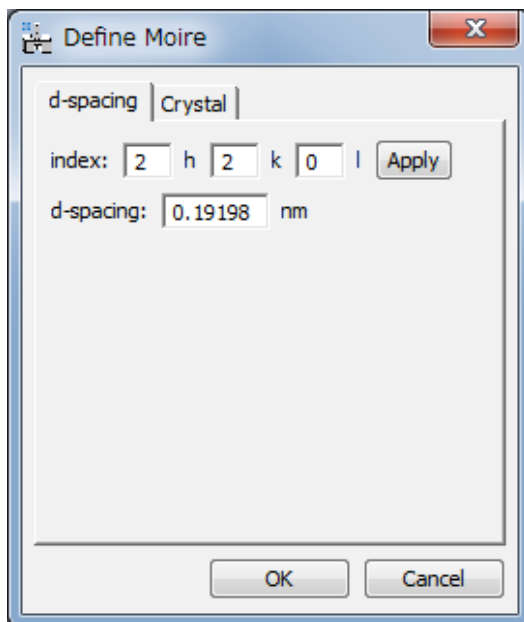


This is a standard Open dialog, so you can browse a directory and select multiple image files. When you choose "Raw data" for Files of type, you can read a binary data. In this case, you have to specify the image size (Width and Height), and Data Type.

## **Define Moire**

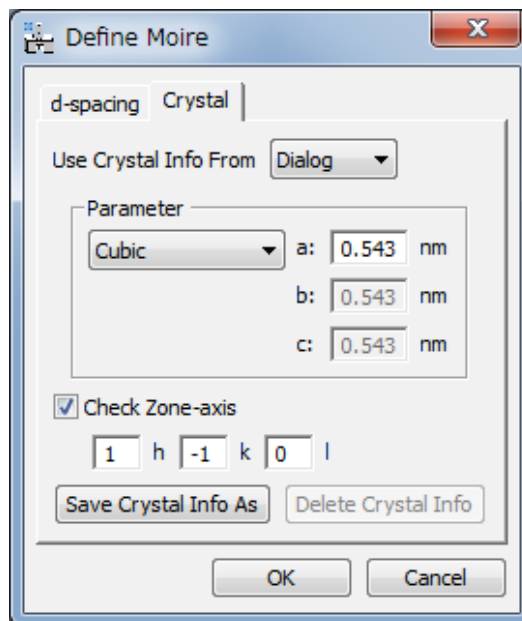
### ***Define Moire Dialog***

#### **d-spacing Tab**



<b>Option</b>	<b>Description</b>
index	Miller indices of the/lattice plane (g-vector) used to obtain the STEM Moiré.
Apply	On click, d-spacing will be displayed.
d-spacing	Lattice plane spacing in nm corresponding to the index. If you want, you can directly input the d-spacing without defining the crystal information.

## Crystal Tab



Option	Description
Use Crystal Info From	Selection of crystallographic information from the current dialog or the saved crystal Info.
Parameter	Defines a crystal system and a unit cell.
Crystal system	Selection of the crystal system from cubic, tetragonal or orthorhombic.
a, b, c	Lattice parameter in nm.
Check Zone-axis	If checked, the diffraction vector (g-vector)/lattice plane index will be checked. If the lattice plane index is not perpendicular to the zone-axis index, the error will be displayed.
Zone-axis	Miller indices of zone-axis normal to the image plane in upward direction (i.e. opposite direction to incident beam).
Save Crystal Info As	You can save the crystal information defined in the current dialog under the specified name.
Delete Crystal Info	Delete the saved crystal Info from the list.

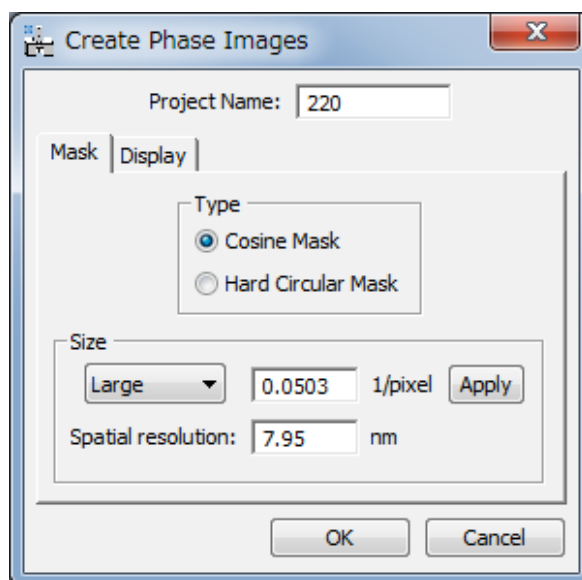
## Phase Calculation Menu

### *Create Phase Image Dialog*

The components of the dialog are described below.

Component	Description
Project Name	Name given to the group of images and results.
Mask Tab	For information about the components of the Mask tab, see <a href="#">Mask Tab</a> below.
Display Tab	For information about the components of the Display tab, see <a href="#">Display Tab</a> below.
OK	Closes the dialog and starts the image calculation according to the specified parameters.
Cancel	Closes the dialog without executing the command.

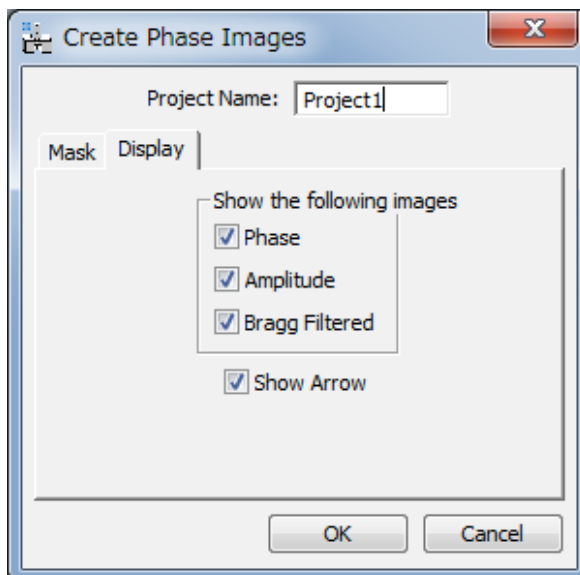
#### Mask Tab



Component	Description
Type	Defines the shape of mask used to isolate the selected spots in the Fourier transform.
Cosine Mask	Half-cosine-shaped mask. Size corresponds to radius of hard cut-off and cosine quarter period (i.e. first zero).
Hard Circular Mask	Circular-shaped mask with a hard cut-off. Size corresponds to radius.
Size	Defines mask radius of hard cut-off (beyond which values are set to zero).
Selection	Default values of large (g/2), medium (g/3) and small (g/4). Custom allows any value.
Text Field	In units of pixels in the FFT.

Apply Button	Displays mask size as circles on Power Spectrum around selected spots (this is just for display purposes and is not necessary for the calculation).
Spatial Resolution	Displays the equivalent averaging in real space (but will appear only if the original image is calibrated).

### Display Tab

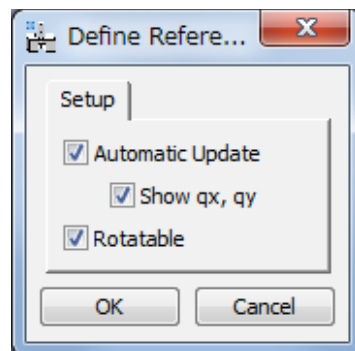


Component	Description
Show the following images	
Phase	Phase image from selected Moiré-spot.
Amplitude	Amplitude image from selected Moiré-spot.
Bragg Filtered	An image without Moiré fringes. Note: This image is required to calculate an average phase image (Average Phase Images).
Show Arrow	An arrow will be shown on original Moiré image in the direction of the g-vector.

**Define Reference Menu**

Refine Setup...
--------------------

Option	Description
Refine	Before running the command, an area needs to be selected by the DM rectangular ROI tool. The command defines this region as the reference lattice and adjusts phase images accordingly (see options). The rectangular ROI can be made rotatable (see Setup).
Setup...	Opens Setup dialog.

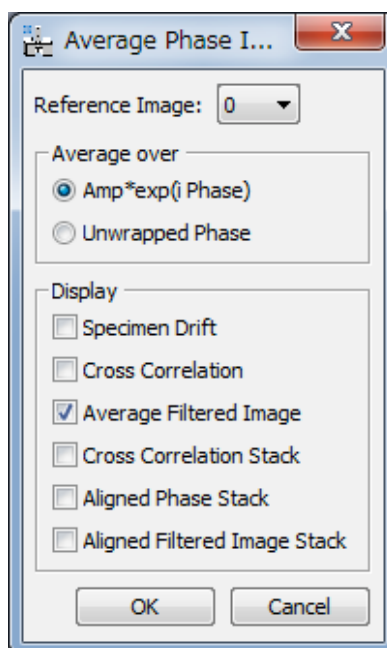
**Setup Dialog**

Option	Description
Automatic Update	Moving the reference area automatically updates the phase images and reference values.
Show qx,qy	Displays the values of the Moiré spot position (qx, qy) in the DM Results window each time the reference area is updated.
Rotatable	Tick to make the rectangular ROI rotatable. Edge length will be adjusted by grabbing the yellow edges, and the rotation angle will be adjusted by the yellow cross (+). (You can change the both edge lengths by dragging the yellow cross when holding down the SHIFT key.)



## Average Phase Images Menu

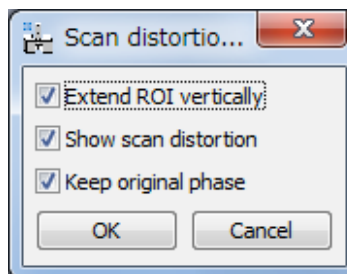
### Average Phase Images Dialog



Component	Description
Reference Image	The phase images will be aligned with respect to the reference phase image specified here.
Average over Amp*exp(i Phase) Unwrapped Phase	Average phase image will be calculated as the phase of the complex sum of Amp*exp(i Phase), or by adding Unwrapped Phases.
Display	
Specimen Drift	If checked, estimated specimen drifts will be displayed.
Cross Correlation	If checked, cross-correlation values will be displayed.
Average Filtered Image	If checked, an averaged Filtered image will be displayed. This image is required to align two phase images for calculating 2D strain.
Cross Correlation Stack	If checked, a stack of cross-correlation maps will be displayed.
Aligned Phase Stack	If checked, the phase images after alignment will be displayed, and you can evaluate the result of alignment using the slice tool.
Aligned Filtered Image Stack	If checked, an aligned Filtered image stack after alignment will be displayed, and you can evaluate the result of alignment using the slice tool.

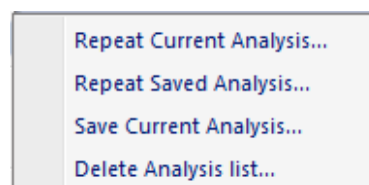
## Scan-line Correction Menu

### Scan-line Correction Dialog

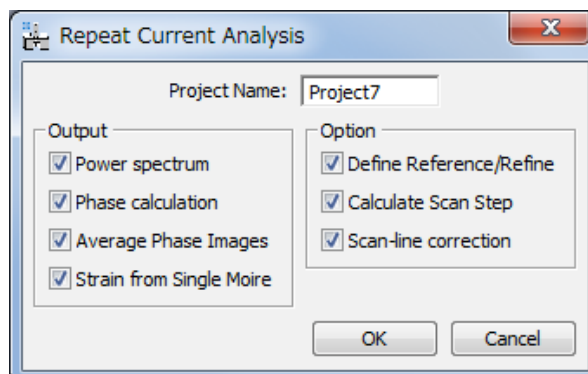


Component	Description
Extend ROI vertically	Scan distortion correction will be measured within the ROI and applied across the whole image from the top to bottom line of the ROI. If checked, the ROI is artificially extended vertically to the top and bottom of the image.
Show scan distortion	If checked, the phase maps (denoted “_SD”) used for the scan distortion correction will be displayed. in addition to the scan-corrected phase images (denoted “_SC”).
Keep original phase	If checked, the original phase images will be kept displayed.

## Repeat Single Moiré Analysis Menu

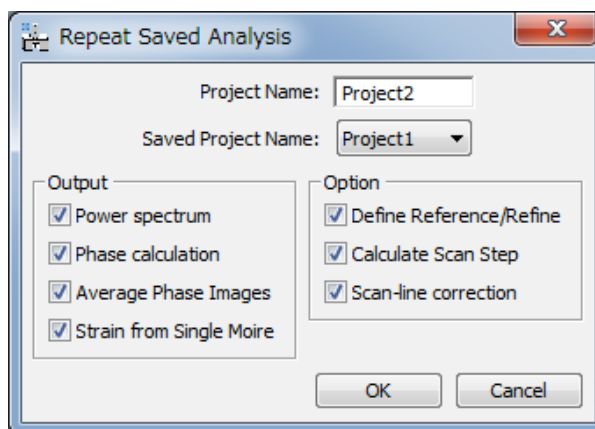


Option	Description
Repeat Current Analysis..	Repeats the same operations as carried out most recent analysis on the front most STEM Moiré images. Note: the current references of the phase images are used to calculate the new phase images. See dialog box for options.
Repeat Saved Analysis...	Repeats the same operations as carried out for a saved analysis on the front most STEM Moiré images.
Save Current Analysis...	Saves the details of the current analysis for later use.
Delete Analysis list...	Removes analyst details from the analysis list.

***Repeat Current Analysis Dialog***

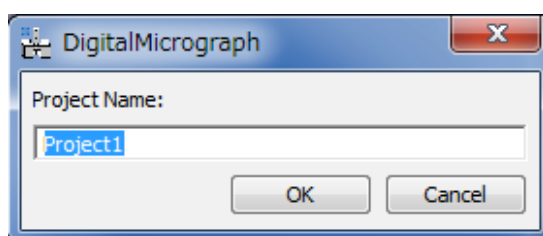
<b>Component</b>	<b>Description</b>
Project Name	Defines the name of the new project.
Output	
Power spectrum	Tick for the power spectrum to be displayed.
Phase calculation	Tick for the phase image to be displayed (including Bragg filtered images if calculated in the repeated project).
Average Phase Images	Tick for the average phase image to be displayed
Strain from Single Moiré	Tick for the strain field to be displayed (if calculated in the repeated analysis).
Option	
Define Reference/Refine	Tick to refine the moiré spot in the same area.
Calculate Scan Step	Tick to refine the scan step during the phase calculation step. If not ticked, the same scan step of the elected analysis will be applied.
Scan-line correction	Tick to apply the scan distortion correction as for the repeated analysis.

### ***Repeat Saved Analysis Dialog***



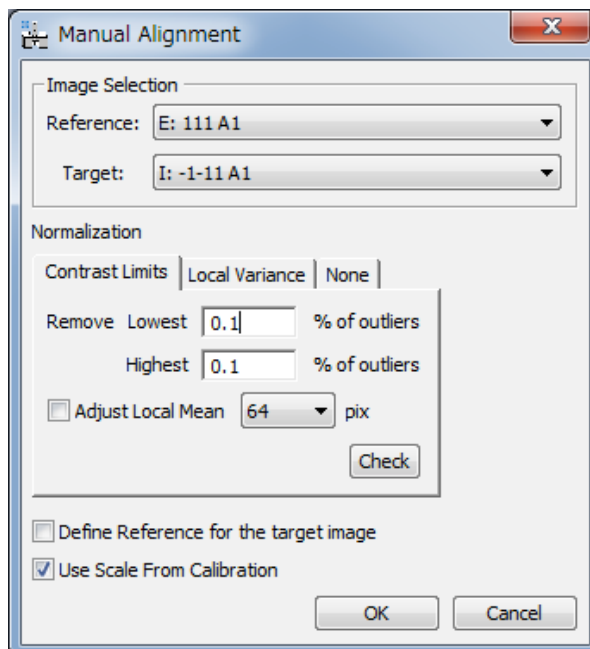
<b>Component</b>	<b>Description</b>
Project Name	Defines the name of the new project.
Saved Project Name	Select the saved project to be used again.
Output	
Power spectrum	Tick for the power spectrum to be displayed.
Phase calculation	Tick for the phase image to be displayed (including Bragg filtered images if calculated in the repeated project).
Average Phase Images	Tick for the average phase image to be displayed
Strain from Single Moiré	Tick for the strain field to be displayed (if calculated in the repeated analysis).
Option	
Define Reference/Refine	Tick to refine the moiré spot in the same area.
Calculate Scan Step	Tick to refine the scan step during the phase calculation step. If not ticked, the same scan step of the elected analysis will be applied.
Scan-line correction	Tick to apply the scan distortion correction as for the repeated analysis.

### ***Save Current Analysis Dialog***



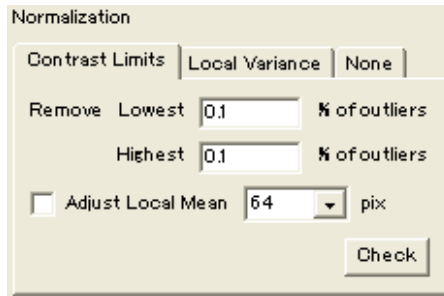
## **Align Two Phase Images Menu**

### **Align Two Phase Images Dialog**



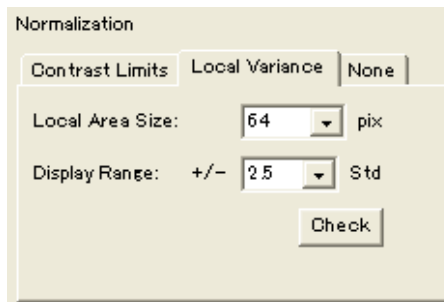
<b>Component</b>	<b>Description</b>
Image Selection	Choice of the two images to be used for alignment (usually Bragg filtered images, in which case the corresponding Phase images will be aligned accordingly).
Reference	Specify the Reference Image i.e. the one which will remain fixed.
Target	Specify the Target Image i.e. the one which will be shifted (magnified and rotated) to align with Reference image.
Normalization (see Scheme Tabs)	Manual alignment tool requires normalized images. Normalization scheme is selected from the Tabs.
Define Reference for the target image	Tick to Define reference in the same area used for the reference image.
Use Scale From Calibration	If checked, the scale (image calibration) of each image will be used Otherwise, the scale will be calculated from the length of Line ROI or Line Annotation.
OK	Closes the dialog and starts the procedure according to the specified parameters.
Cancel	Cancels the procedure.

**Normalization**  
**(Contrast Limits Tab)**



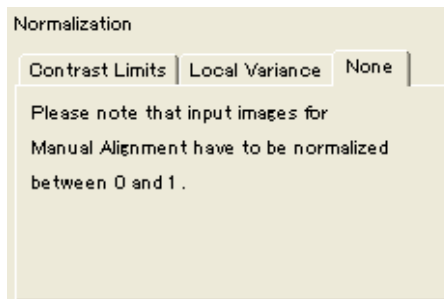
Component	Description
Remove outliers	Display limits (Lowest and Highest values) are defined by excluding the specified % of outliers (same as DM display limits).
Adjust Local Mean	Tick to adjust background using the local mean. The size of area used to calculate the local mean is specified in pixels.
Check	Click to check the effect of normalization.

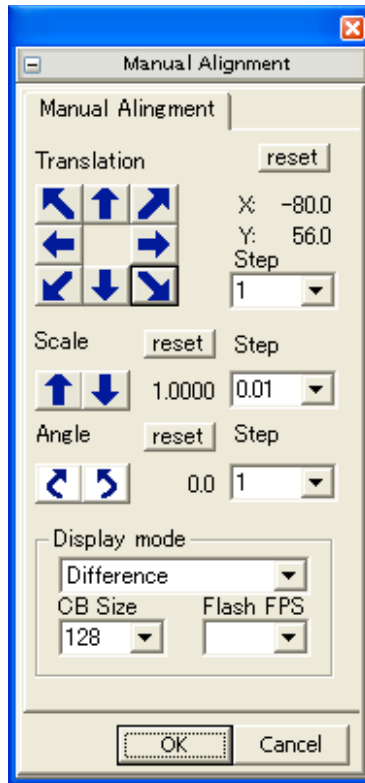
**Normalization**  
**(Local Variance Tab)**



Component	Description
Local Area Size	Specifies a local area size in pixels.
Display Range	Specifies display range in terms of local standard deviation (std). Namely, the display range will be <local mean> +/- <display range>*<local std>.
Check	Click to check the effect of normalization.

**Normalization**  
**(None Tab)**



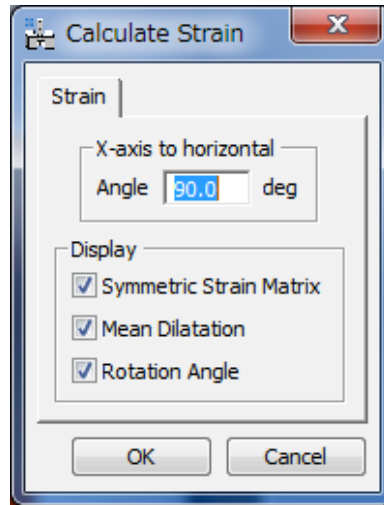
***Manual Alignment Tool***

Component	Description
Translation	Translates the Target image with respect to the Reference image, in the direction of the arrow clicked upon. Keyboard arrow keys can also be used.
Reset	Returns the target image to its initial position.
Step	Step for one click in pixels.
Scale	Magnifies (or demagnifies) the Target image with respect to the Reference image.
Reset	Returns the Target image to its initial magnification.
Step	Step for one click in fractions of scale change.
Angle	Rotates the Target image, clockwise or anticlockwise, with respect to the Reference image.
Reset	Returns the Target image to initial orientation.
Step	Step for one click in degrees.
Display mode	Display mode may be selected from the pull-down list.
CB Size	Defines the checker board size (in pixels) for Checker Board display mode CB.
Flash FPS	Defines Image flash rate (in seconds) for Flash mode display. (Actual flash rate is hardware dependent.)



## Calculate 2D Strain Menu

### Calculate Strain Dialog



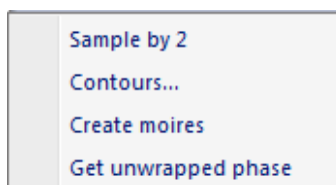
Component	Description
X-axis to horizontal	Defines the orientation of the x-axis used for calculating the strain tensor components. Angle defined from the image horizontal to the desired x-axis (in degrees, anticlockwise positive). The values used for the previous calculation will be shown.
Angle	Allows angle to be defined manually.
Display	Choice of results to be displayed.
Symmetric Strain Matrix	Images of $\epsilon_{xx}$ , $\epsilon_{yy}$ and $\epsilon_{xy}$ to be displayed.
Mean Dilatation	Image of $\delta_{xy}$ to be displayed (average of $\epsilon_{xx}$ and $\epsilon_{yy}$ ).
Rotation Angle	Image of $\omega_{xy}$ to be displayed. Values in degrees and anticlockwise positive.

**Phase Maths Menu**

A	dd constant phase
R	enormalise phase
A	dd phase images
S	ubtract phase images
I	nvrt phase

<b>Option</b>	<b>Description</b>
Add constant phase	Adds a uniform phase value to the front most image and renormalizes the phase.
Renormalize phase	Renormalizes the phase between $-\pi$ and $+\pi$ .
Add phase images	Adds two phase images together (requested in a dialog box) and displays result in a third window (after phase renormalization). If the phase images have been aligned, the new phase image will have a reference equal to the sum of the references of the two phase images. Otherwise, the new phase image will have a reference equal to the first phase image selected.
Subtract phase images	Subtracts two phase images (requested in a dialog box) and displays result in a third window (after phase renormalization). If the phase images have been aligned, the new phase image will have a reference equal to the difference of the references of the two phase images. Otherwise, the new phase image will have a reference equal to the first phase image selected.
Invert phase	Calculates the negative of the phase (and inverts the g-vector).

## Phase Tools Menu



Option	Description
Sample by 2	Rebins the front-most phase image by two and multiplies the reference by two (thus preserving the reference values $g_x$ and $g_y$ in $\text{pixels}^{-1}$ of the newly sampled image).
Contours	Superimposes contours on the front most image (see options).
Create moirés	Creates a moiré image from the front most phase image. Asks for the magnification factor $n$ equivalent to moiré fringes every $n$ lattice fringes.
Get unwrapped phase	Displays unwrapped phase image in new window. Note: there is no unique solution for phase unwrapping.

## Contours dialog (Option Tab)



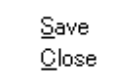
Component	Description
Contour spacing	Step in image values between each contour.
Number of contours	Total number of contours displayed.
Mid contour	Image value corresponding to mid contour.
Contour width	Contour line width in pixels.

## Extract Rotated Region Menu



Option	Description
Define	Before running the command, an area needs to be selected by the DM rectangular ROI tool. The rectangular ROI will be made rotatable. Note: Edge length can be adjusted by grabbing the yellow edges, and the rotation angle by adjusting the yellow cross (+). (You can change the both edge lengths by dragging the yellow cross when holding down the SHIFT key.)
Extract	Extracts the region within the ROI. The long edge direction will be rotated to horizontal.
Extract Group	Extracts the same area from a group of images (e.g. strain maps).

## Image Group Menu



Component	Description
Save	Saves (with dialog) all images of the same type as front-most image (e.g. strain maps).
Close	Closes (without saving) all images of the same type as the front most image.