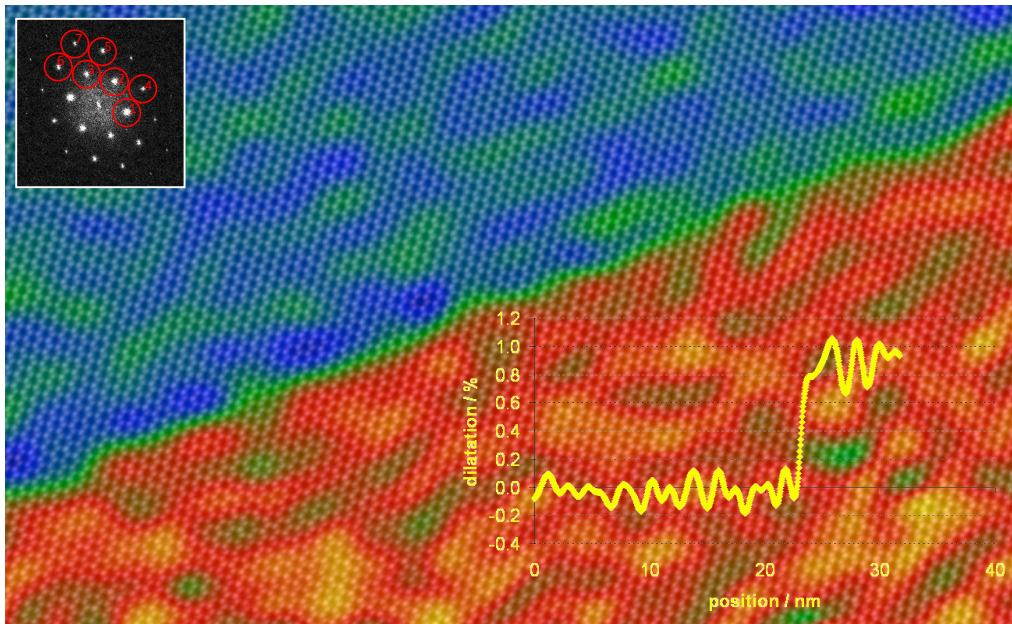# *GPA for DigitalMicrograph*

Geometric Phase Analysis

GPA Phase Manual 4.12

HREM Research Inc.

Conventions

The typographic conventions used in this help are described below.

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

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Introduction to GPA

Welcome to the GPA Phase. DigitalMicrograph plug-in for strain mapping from high-resolution transmission electron microscope images (HRTEM), high-resolution scanning transmission electron microscope images (STEM), or indeed any type of lattice image. The main reference for the theory is:

> M. J. Hÿtch, E. Snoeck and R. Kilaas, Ultramicroscopy 74 (1998) 131–146. *Quantitative measurement of displacement and strain fields from HREM micrographs*

and additionally:

> F. Hüe, C.L. Johnson, S. Lartigue-Korinek, G. Wang, P.R. Buseck, M.J. Hÿtch, J. Electron Microscopy 54 (2005) 181-190. *Calibration of projector lens distortions.* doi:*10.1093/jmicro/dfi042*.

> M. J. Hÿtch and T. Plamann, Ultramicroscopy 87 (2001) 199–212. *Imaging conditions for reliable measurement of displacement and strain from high-resolution electron microscope images*.

Applications of GPA can be found in the following:

[1] F. Hüe, M.J. Hÿtch, H. Bender, F. Houdellier, and A. Claverie, Phys. Rev. Lett. 100 (2008) 156602. *Direct mapping of strain in a strained-silicon transistor by high-resolution electron microscopy. doi:10.1103/PhysRevLett.100.156602*.

[2] C.L. Johnson, E. Snoeck, M. Ezcurdia, B. Rodríguez-González, I. Pastoriza-Santos, L.M. Liz-Marzán, and M.J. Hÿtch, Nature Materials 7 (2008) 120-124. *Effects of elastic anisotropy on strain distributions in decahedral gold nanoparticles. doi:10.1038/nmat2083*.

[3] M.J. Hÿtch, J.-L. Putaux, J. Thibault, Phil. Mag. 86 (2006) 4641–4656. *Stress and strain around grain-boundary dislocations measured by high-resolution electron microscopy. doi:10.1080/14786430600743876*.

[4] J.L. Taraci, M.J. Hÿtch, T. Clement, P. Peralta, M.R. McCartney, J. Drucker and S.T. Picraux, Nanotechnology 16 (2005) 2365-2371. *Strain mapping in nanowires. doi:10.1088/0957-44/16/10/062*.

[5] M. J. Hÿtch, J-L. Putaux, J-M. Pénisson, Nature 423 (2003) 270-273. *Measurement of the displacement field around dislocations to 0.03Å by electron microscopy. doi:10.1038/nature01638*.

Software requirements

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

- DigitalMicrograph (GATAN^{TM})
- USB Key Driver
- HREM Mouse Tool Plug-in (Free-ware downloadable from www.hremresearch.com)
- IPU Plug-in (Free-ware downloadable from 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 GPA, or you can find it on our web site.

Installing GPA 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, GPA menu commands will appear under "GPA Phase" 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.
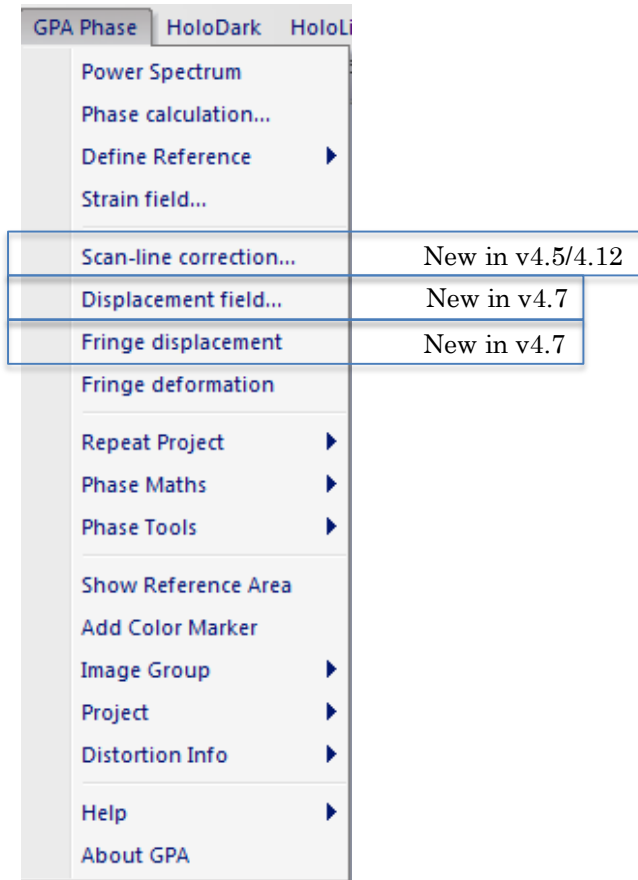
Installing IPU Plug-in
GPA uses some functions based on the Intel' MKL (Math Kernel Library) provided by the IPU plug-in. All the files relating the IPU plug-in can be installed by drag-and-drop copy. Please consult the ReadMe file that comes with the IPU plug-in.

In this manual, we will dive straight into the use of the GPA Phase 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. *GPA Phase 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 GPA variables will not be transferred.

2. *All the commands related to GPA Phase* are located in the menu **GPA Phase**:

Scan-line correction...	New in v4.5/4.12
Displacement field...	New in v4.7
Fringe displacement	New in v4.7

3. The *only other additional feature* to DigitalMicrograph is located in the *Standard Tools* Window:
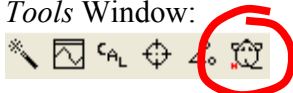
This **mouse tool** is a regular feature of other *HREM Research* plug-ins and is used in GPA Phase only for the selection of spots in the *Power Spectrum*, as we will see.

New features in version 4.7

It might seem ironic but we have waited for the version 4.7 to include the direct determination of displacement fields from phase images. There are two main reasons for this. The first is that most people are interested in strain measurements, and these are most accurately determined directly from the phase images. The second, more technical reason is that phase unwrapping is necessary to determine the displacement field and there is no unique solution to phase unwrapping in two dimensions. We have had to make a compromise.

Here are the two new functions:
- **Fringe displacement.** Displacements perpendicular to a *single* set of lattice fringes are determined, either in pixels if the image is not calibrated or in nm for calibrated images.
- **Displacement field.** The full 2D vector displacements in the plane of the image are determined from 2 phase images.

These commands are the natural partners to **Fringe deformation** and **Strain field** respectively.

New features of version 4.5

We have included in GPA 4.5 a new feature:

- **Scan distortion correction.** STEM images are plagued by distortions due to the scan. These distortions are random and therefore cannot be corrected from a reference image, unlike CCD distortions or projector lens distortions for HRTEM images. Several ways have been proposed to correct them. In GPA 4.5, we have implemented a simple routine to correct "fly-back" distortions: the rigid displacements of a whole scan lines.

New features of version 4.0

GPA Phase 4.0 has the possibility of calculating strain maps from multiple, i.e. more than two, phase images:

- **Multi-phase strain maps**. In principle, strain maps can be calculated from just two phase images. For previous versions of GPA, we typically chose the phase images from the two strongest spots in the Power Spectrum. But if many viable spots are available (notably for aberration-corrected HRTEM images) it is a pity to miss the extra information. A routine has therefore been implemented in v4, which allows you to calculate the strain maps from as many phase images as you like. The strain maps are a result of a least-squares fitting procedure and aims to improve the signal-to-noise ratio of the measured strain. See the Additional Functions section for details.

This is the first time we have updated the basic **Strain field…** routine since the original version of GPA, so we thought it worth a version change!

To know more about the idea behind using multiple phase images see:
A. K. Gutakovskii, A. L. Chuvilin, and S. A. Song, Bulletin of the Russian Academy of Sciences: Physics 71 (2007) 1426–1432. *Application of high-resolution electron microscopy for visualization and quantitative analysis of strain fields in heterostructures*.

New features of version 3

GPA Phase 3.0 can handle the complex image, which will be obtained by using electron hologram or an exit wave reconstruction procedure.
Additional features include:

- **Polynomial fit to Lens distortion correction**. Lens distortion is normally changes slowly, and can be expressed by polynomial function. Thus, a polynomial fitting will reduce random noise in the lens distortion pattern.
- **Rotatable ROI**. In some case you may want to use the reference rectangle area that is not parallel to horizontal or vertical direction. Now, after placing a regular rectangle ROI to show the size you want, you can rotate the rectangle ROI as well as change the size.
- **Color marker**. The intensity scale can be added to images (for example, deformation maps) in the form of a color bar, including minimum and maximum values.

New features of version 2

GPA Phase 2.0 is faster and more user friendly than GPA Phase 1.0. In addition, there are a number of new features, such as:

- **Calibrated images**. If the analysed image has a calibrated scale (in nm, for example), all phase results will be calibrated accordingly (even when binned, see below). More

importantly, the spatial resolution of the results will be indicated when defining the mask size in **GPA Phase...Calculate Phase**.

- **Image binning**. The resulting phase image can be chosen to have a reduced size (in pixels) with respect to the original image, using the binning option in **GPA Phase...Calculate Phase**. Analysing a 2048 by 2048 pixel image at binning 4 will produce results 512 square. This speeds calculations and liberates space. No information is lost, as the mask used in Fourier space is always much smaller than the original picture size.

- **Automatic distortion correction**. Previously, a reference image had to be analysed manually each time the phase images were to be corrected. Now, this is done automatically. The reference image (distortion information) just needs to be analysed once and saved using the menu **GPA Phase...Distortion Info**. All subsequent phase analyses can then call up and automatic correction using the **Distortion** tab in **GPA Phase...Calculate Phase**.

- **Repeat phase project**. All the operations carried out during a phase project can be repeated on a new image with just one click using **GPA Phase...Repeat phase project**, including strain fields. This means of course that the reciprocal lattice vectors need to be roughly the same as before. This command is ideal for analysing a series of images of a specimen.

GPA Phase Tutorial

Getting Started

Open the image "GPA Test 0" using the DM command **File…Open** from the GPA Phase Manual folder:
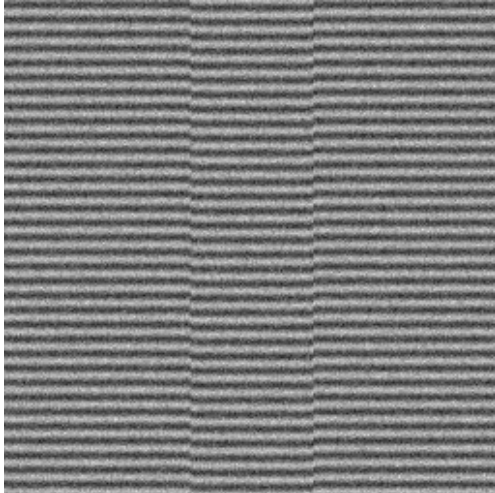
Technical note: you can find out how this image was created by looking at the script "GPA Test image 0.s" in the Phase Manual folder. Indeed, you can play with the image by changing the script, in particular the variable *dPhase* which determines the displacement.
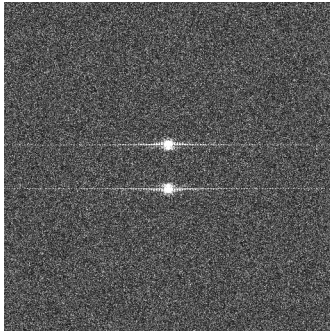
Hint: to run a script in DM, press CTRL-ENTER.

The first step in phase analysis is to calculate the *Power Spectrum* of the image:
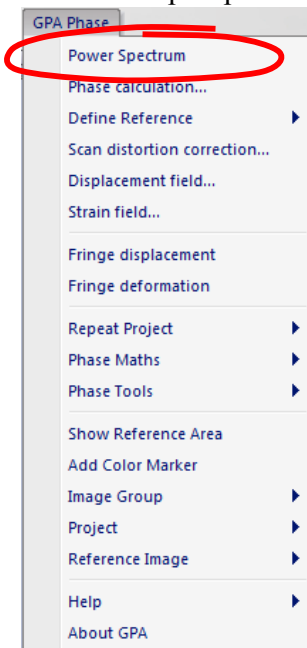
Technical note: in GPA, the image does not have to be a power of two in size (e.g. 512 by 512). However, streaks may appear in the power spectrum if greatly different in size from a power of two.

You will see an image similar to this:

Technical note: the power spectrum is the modulus squared of the Fourier transform of the image. People are often surprised by the lack of a central spot in the power spectrum but this is normal for images where the mean intensity is zero, an important difference with diffraction patterns. The horizontal streaking of the spots is due to the interfaces in the image and is not, in this case, an artefact.

Now choose the **mouse tool**: and click on one of the spots.

Why not zoom in using the DM **magnifying glass** tool:
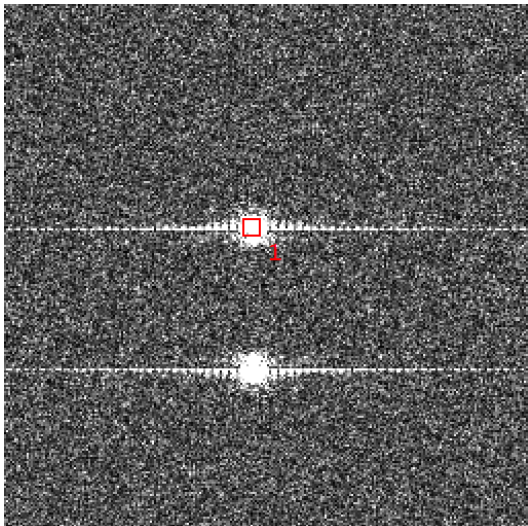
Technical note: do not worry about "hitting" the spot exactly. GPA will automatically hunt locally for the maximum intensity in the spot, even though the red square marks the actual pixel you hit.

Hint: if you wish to delete your mark, click on the mouse mark again with the SHIFT key down, or use the DM **arrow tool** to select and delete.

For the moment we want only one spot marked, but GPA can deal with multiple selections, as we will see later. The chosen reciprocal lattice vector will be referred to as **g**.

We are now ready to calculate our first *Phase Image*:

The following dialogue box will appear:
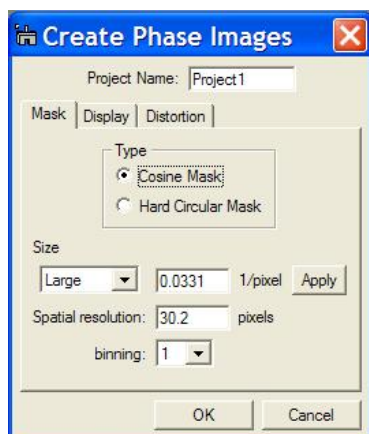
Technical note: the choice of the mask type (shape) is not that critical though the hard circular mask is to be avoided (only included for completeness). Hard masks in Fourier space introduce rippling effects in real-space, which is why smooth masks are preferred. Mask size is the most important parameter.

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. 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 = g/4), medium (g/3) to large (g/2). As you do this, the result of your choice will be seen on the *Power Spectrum*:
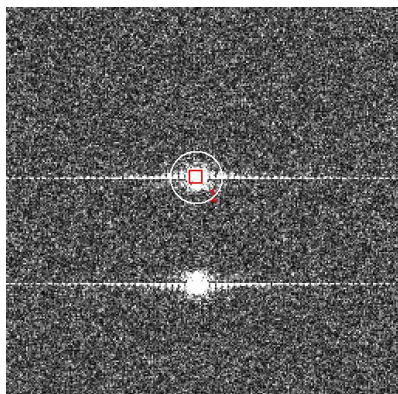

Technical note: the radius of the mask shows the area selected in Fourier space around the spot of interest. Decreasing the mask radius will produce smoother results but with less spatial resolution. The maximum recommended size is g/2 corresponding to the large mask size.

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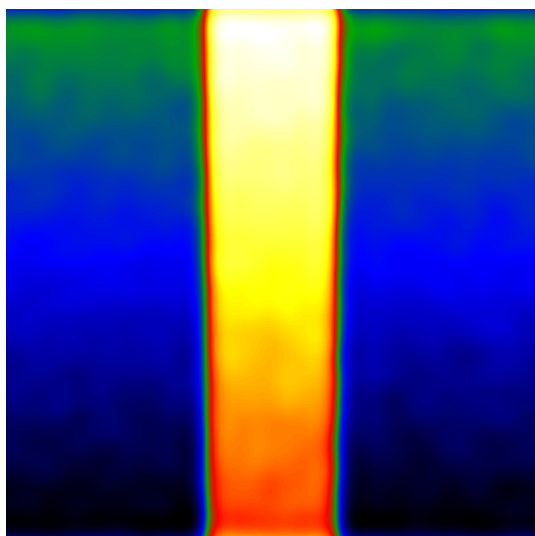
Technical note: GPA uses the temperature colour scale for displaying image values. If you prefer grey scales use the DM menu **Object…Image Display…Color**. Similarly, if you wish to change the maximum and minimum display values use DM menu **Object…Image Display…Contrast** or select an area on the histogram.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

This phase image has values in radians from –π to +π. The next step is to define area which will correspond to the reference lattice. Use the DM **ROI tool** (region of interest tool) to select and area:
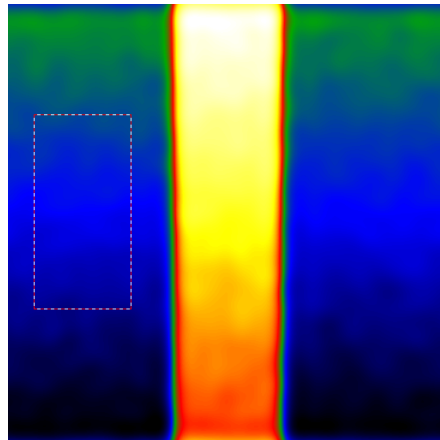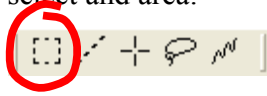

Technical note: choose an area of undistorted lattice as your reference area, recognised in the phase image as an area of uniform contrast or uniform gradient. For example, do not choose an area which straddles the interfaces. Having said that, please experiment.

and choose the next GPA phase command **Define Reference**.
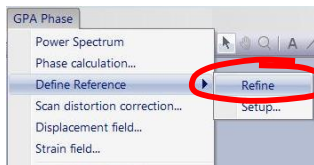
Hint: if you do not like the reference area, just grab and slide the ROI across the image. GPA will automatically update the reference area. This function can be deactivated in **Define Reference…Setup**.

The result will be the following:
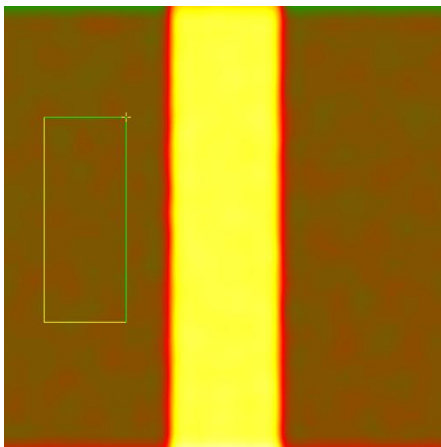
Technical note: if you want to know the actual values of the reference lattice $\mathbf{g}=(g_x,g_y)$ then look in the DM *Results Window*, and if necessary apply **Define Reference…Setup…Show gx, gy**. Values are in pixels^{-1}

The phase image now has a well-defined reference lattice and can be interpreted. The uniform area of phase shows that the lattice is identical to the reference (here in brown). The change in the relative phase shows that the central band (here in yellow) is displaced with respect to the reference. You can see this on the original image. This is the basis of the geometric phase technique: the measurement of displacement of lattice fringes.

By choosing the DM **profiling tool**, the phase shift can be visualised:
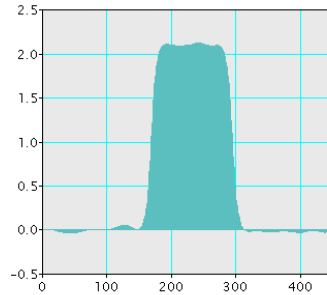
In the reference area the phase is zero and in the central band takes a value of 2.2 radians. This value can be verified in the original script used to create the image "GPA Test image 0". Now choose the reference area in the central band, and you will see that the displacement is reversed. This illustrates the overall principle:

> Only *relative* phase shifts are important and all measurements refer to the particular *reference* lattice used.

Fringe displacements

From theory, geometric phase is related to displacement by the following equation:

$$P_g(\mathbf{r}) = -2\pi\mathbf{g}.\mathbf{u}(\mathbf{r})$$

where $P_g(\mathbf{r})$ is the geometric phase of a set of lattice fringes with reciprocal lattice vector $\mathbf{g}$, $\mathbf{u}(\mathbf{r})$ is the displacement and $\mathbf{r}$ the position coordinate in the image. This can be further simplified if we consider only displacements perpendicular to the fringes, u_g, and that the fringe spacing, d, is equal to 1/ g:

$$P_g = -2\pi u_g / d$$

In terms of displacement this means that:

$$u_g = -\frac{P_g}{2\pi} d$$

i.e. the phase in units of 2π gives the displacement as a fraction of the lattice spacing. A phase shift of 2.2 radians represents a displacement of $-2.2/2\pi = -0.3501$ of a lattice spacing. As a new feature of version 4.7, these relations have been programmed for you.

Select the phase image as the upper-most image and choose **Fringe displacement…** from the main menu:

> **Note:** the command **Displacement field…** for the measurement of 2D displacement fields will be detailed at the end of the manual.

You should see the following result:

Phase   Fringe displacement
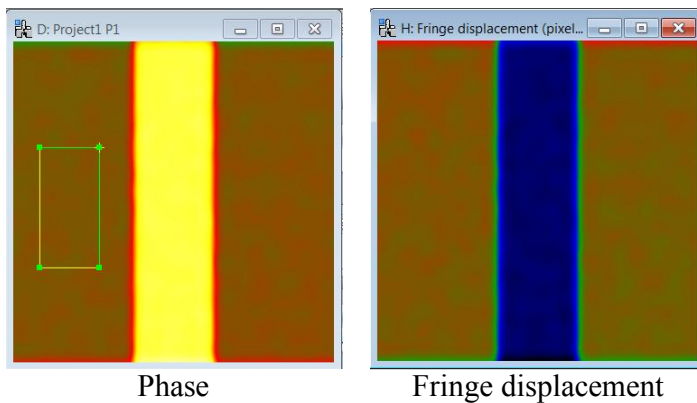
Note: the colour change between the phase and the displacement image is due to the negative sign in the phase-displacement equation.
Look back to the original fringe image and you will see that the fringes are displaced in the negative g-direction (here, the g-direction is upward).

You might like to take a profile across Fringe displacement image to look at the actual values:
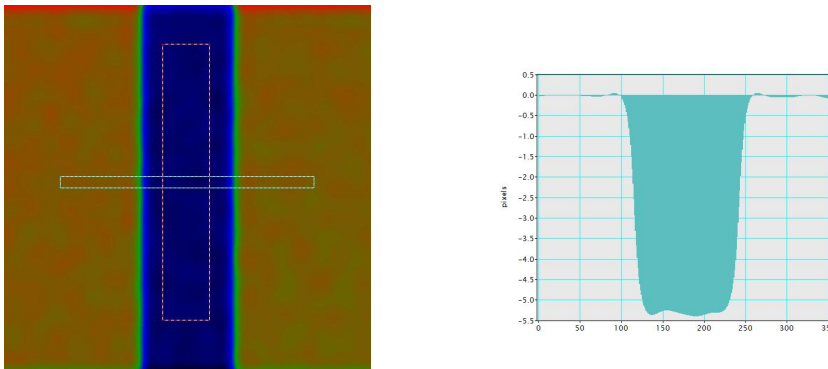
Since the original image is not calibrated (in nm/pixel) the displacement is given in pixels. Given the fringe spacing was 15 pixels, the exact displacement should be -5.252 pixels.

As you can see from the profile, the result is not exactly this value: there are fluctuations. These come from the fact that noise was added to the original simulated image to make it look more realistic. Delineate a rectangular ROI and use the DM function **Analysis…Statistics… Mean and Std. Dev**. You will obtain the result in the Output window, something like Mean = -5.278 pixels, Standard Deviation = 0.0522 pixels.

In the presence of *noise* exact values are never obtained: there will always be an *uncertainty*, quantified by the standard deviation. One hopes that the true value is within the range of uncertainty…

Fringe deformation mapping

Most people are interested in measuring deformation and strain, so let us move quickly on from the phase images and displacement. Open the image "GPA Test 1":
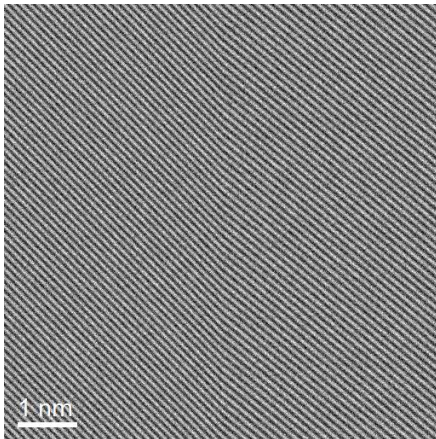
A cunning distortion of the fringes is hidden in this image. To measure this distortion the routine as ever is to produce a phase image with a well-defined reference. Here is a typical result:
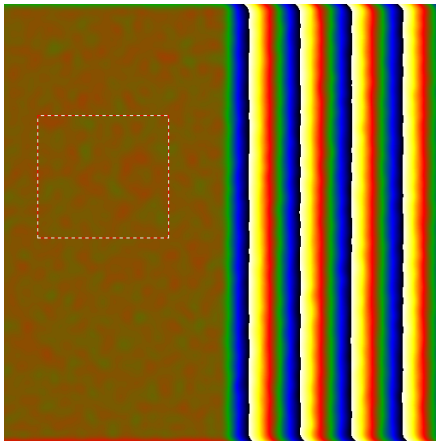
Technical note: do not worry about the "phase jumps" i.e. where the phase suddenly goes from black to white. This is quite normal and results from the normalisation of the phase between $-\pi$ and π. Imagine the phase going round a circle moving seamlessly from 0 to π to $-\pi$ and back again. No discontinuity is present in the underlying lattice images.

The abrupt change in gradient of the phase from one side to the other is witness to the deformation. Let GPA calculate this deformation from the phase image using **Fringe Deformation**:
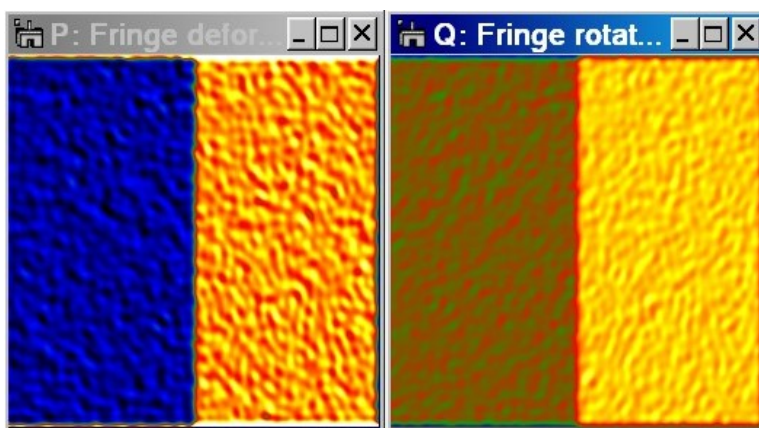

The first image shows the change in lattice spacing relative to the reference lattice in fractional units (i.e. 0.02 means 2% expansion). The paired image shows the rotation of the lattice fringes with respect to the reference in degrees (in-plane rotation of course) and positive anticlockwise. By default the minimum and maximum values are (±5% deformation and ±5° rotation). Now the deformation and rotation can be visualised by taking profiles or measured in ROI boxes using DM **Analysis…Statistics…Mean and Std. Dev**.

Precision and Spatial Resolution

GPA allows the visualisation of lattice deformation. In the previous example, we can clearly see that the image is divided neatly into two regions. On the left, lattice fringes with a particular lattice spacing and orientation and on the right, lattice fringes expanded and rotated with respect to this lattice (or vice-versa, if the reference lattice was chosen on the right). GPA is much more than this, however, it is a tool for measuring deformation. Deformation can be measured using the profile tools and statistical tools in specified areas, as has been seen. Each pixel in the image is also a measure of the local deformation and lattice orientation. The question is how local and how precise?

It is not possible to give a general theoretical answer to this question. An experimental way of estimating will be given here: the standard deviation of the fluctuations in a uniform part of the lattice gives the *precision*, and the length scale of these fluctuations gives the *spatial resolution*. The fluctuations are assumed to be due to noise, of course. The standard deviation is easily measured using the DM command **Analysis…Statistics…Mean and Std. Dev**.

The *spatial resolution* depends on the mask size used in the analysis. Did you spot the new feature of GPA 2.0 when creating the phase image for GPA test 1?
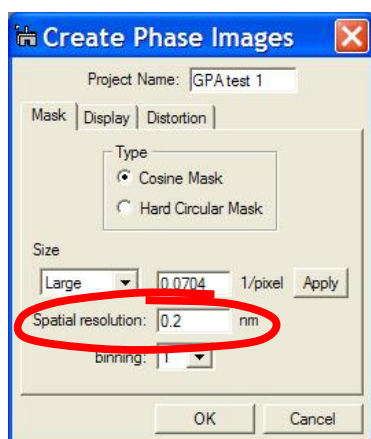
Technical note: If the original image was not calibrated, the spatial resolution is displayed in pixels. If you recalibrate the original image, you need to recalculate the Power Spectrum.

Hint: To calibrate an image using DM draw a line, of which you know the length in nm, using the DM ROI tools. Then use Analysis/Calibrate... To show the scale bar use Edit/Data Bar...

In this case, the spatial resolution of the results will be 0.2 nm. We also provide the radius of the FFT mask, κ in pixels^{-1}, which gives a spatial resolution of $1/\kappa$ in pixels. Changing the mask size will change the spatial resolution (updated automatically).

The precision is a direct function of the noise in the image. Double the amount of noise by modifying the original script "GPA Test image 1" and see the results. Similarly, the spatial resolution is a direct function of the *Mask size* used in the GPA analysis. Repeat the experiment with a smaller mask. Notice that the precision has increased but the spatial resolution has decreased. This is an essential feature of local measurements: precision is inversely related to spatial resolution.

When quoting results from GPA, always quote the ***precision*** at a certain ***spatial resolution***.

Determining strain tensors

In order to measure 2-D strain tensors, two sets of lattice fringes are necessary in the image, as in the image "GPA Test 2":
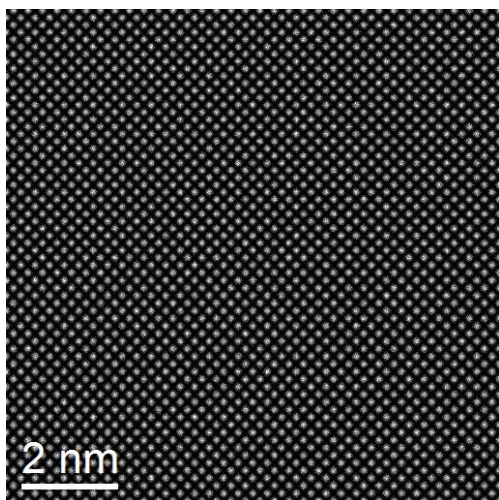

> **Technical note:** a deformation is indeed present here, see the script "GPA Test image 2".

Two phase images are needed to calculate strain, and to do this two spots in the *Power Spectrum* can be selected at once.
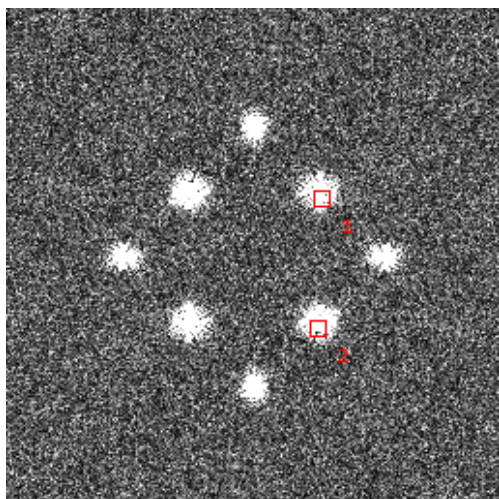

> **Technical note:** in principle, it does not matter which two spots you choose, so long as their g-vectors are not parallel. In practice, the highest precision is obtained with low order spots and ones nearest to right-angles with respect to each other. Spots absent in the crystal structure are to be avoided (e.g. present due to double diffraction, misalignment etc.).

Carry out **Phase Calculation** and notice that a mask is placed around both spots in the *Power Spectrum*. Choose a project name of "Test 2" and the results will look like the following:
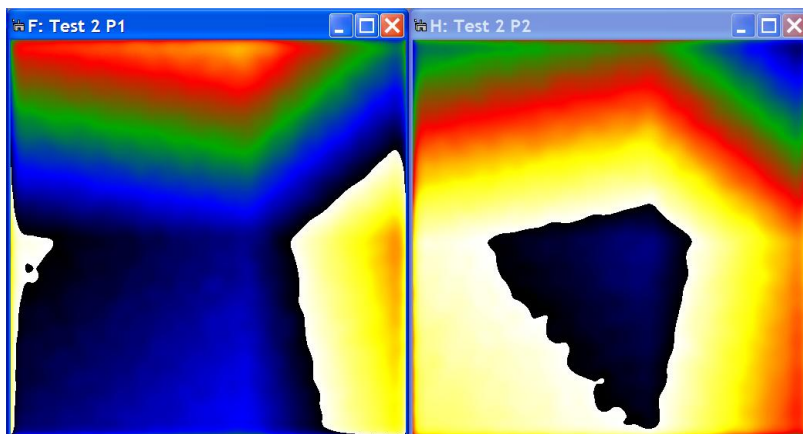
As previously, a reference lattice needs to be defined. This is done by defining an area with the DM **ROI tool** on one of the phase images exactly like the previous examples:
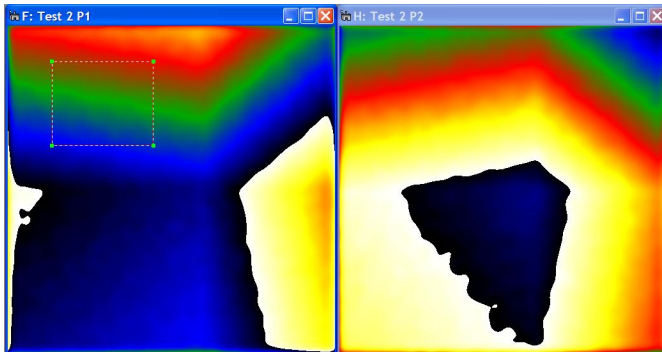

Hint: it is not always easy to recognise a good reference region. Just go ahead and try, and if necessary change the selection. Usually the situation becomes clearer after calculating the strain field.

When the **Define Reference** command is used, GPA will automatically redefine the reference area on all of the phase images in the group (here, two phase images):
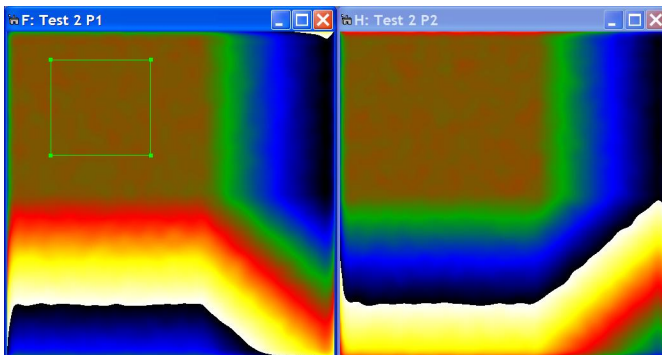
Technical note: it is important for consistency to have the same area of crystal acting as a reference. This feature can be deactivated in **Define Reference…setup**.

The strain tensor can now be determined with the command **Strain field...**. When asked, select the above two images "Test 2 P1" and "Test 2 P2" for the calculation (default values are the two most recent images). In the next dialogue, the angle requested corresponds to the direction of the *x-axis* with respect to the horizontal (angles anticlockwise positive):
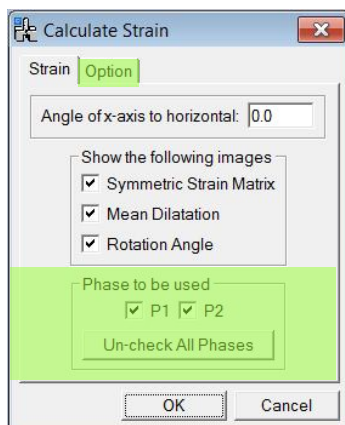
Hint: if a ROI line tool is marked on the original image, the default value will be parallel to this line.

Green areas: new features in GPA 4.0. See later for details.

Choosing the *x-axis* parallel to the picture horizontal axis (i.e. angle zero) and selecting symmetric strain matrix, dilatation and rotation, the following image group will be obtained:
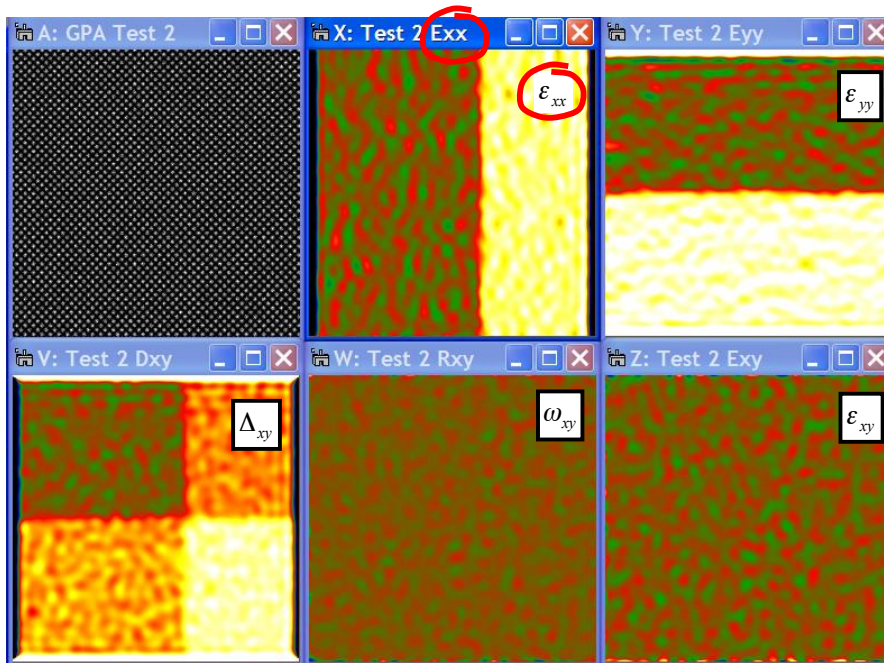
Technical note: strains as fractions (e.g. 0.02 equivalent to 2% strain) and angles in degrees (anticlockwise positive). Default colour range is ±5% strain and ±5° rotation.

This is the final results of GPA strain analysis: the complete 2-D strain tensor. Now it is your job to enjoy and interpret the results!

Additional functions

## Strain field calculation with multiple phase images (v 4.0)

In principle, only two phase images are necessary to calculate the 2D strain tensor, and in previous versions of GPA (up to v3), strain measurements were performed by selecting the two phase images with the highest signal-to-noise ratio. However, experimental phase images are noisy, so it is maybe interesting to be able to combine the information from more than 2 phase images. Indeed, now that aberration-corrected HRTEM is more widely available, the number of useful reflections in the power spectrum has increased significantly. Take a look at the following example from an image called *GPA SiGe SACTEM*:
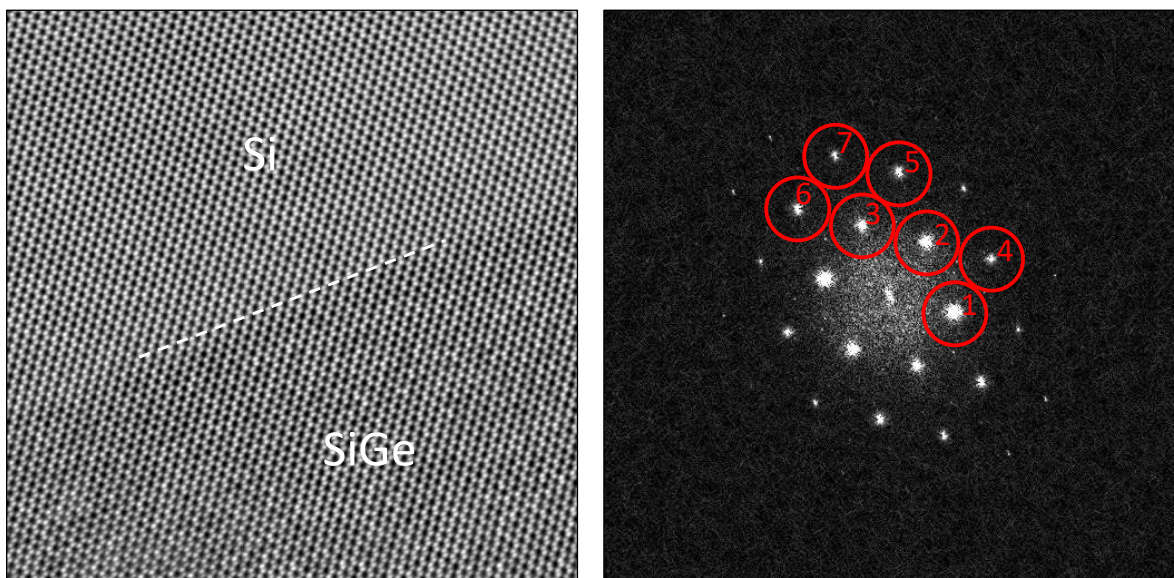
This image was taken on the aberration-corrected SACTEM microscope in Toulouse of SiGe grown epitaxially on a Si substrate [F. Houdellier & M.J. Hÿtch, Microelectronic Engineering 84 (2007) 460–463]. Select the 7 spots circled in the power spectrum with the **mouse tool** and calculate the amplitude and phase images. Use the **large mask size** and try and use the spots in the order indicated above. You should find the following images displayed after defining a reference area:
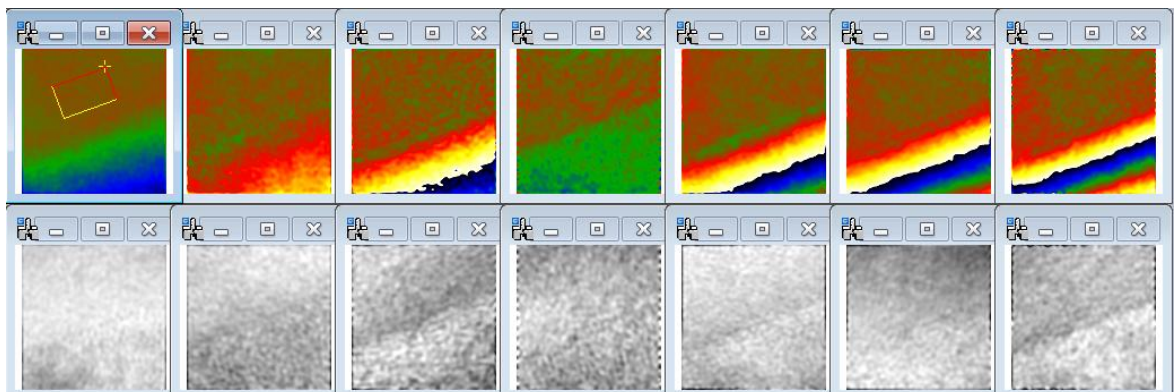
Now calculate the strain map:
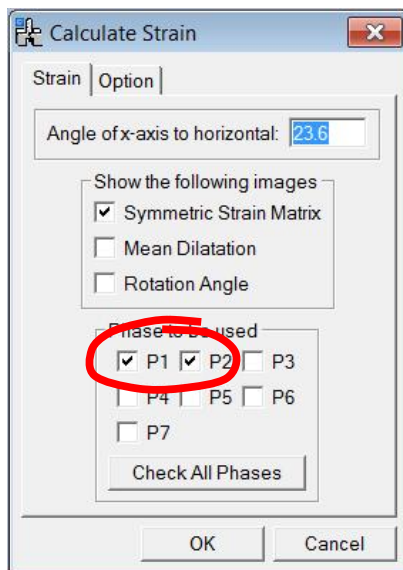
Hint: You can define the direction of x-axis by a Line ROI on the original image. Then, the angle of x-axis to horizontal is automatically read from the line ROI.

Hint: the default phase images are the two topmost phase images in DM. Check and uncheck the boxes as you like.

By default, strain will be calculated from two phase images, as shown. The default phase images will be the topmost two phase images in DM, so tick and untick boxes if necessary to choose P1 and P2 as shown. Verify that the x-axis is parallel to the interface and calculate the symmetric strain matrix by clicking on OK:
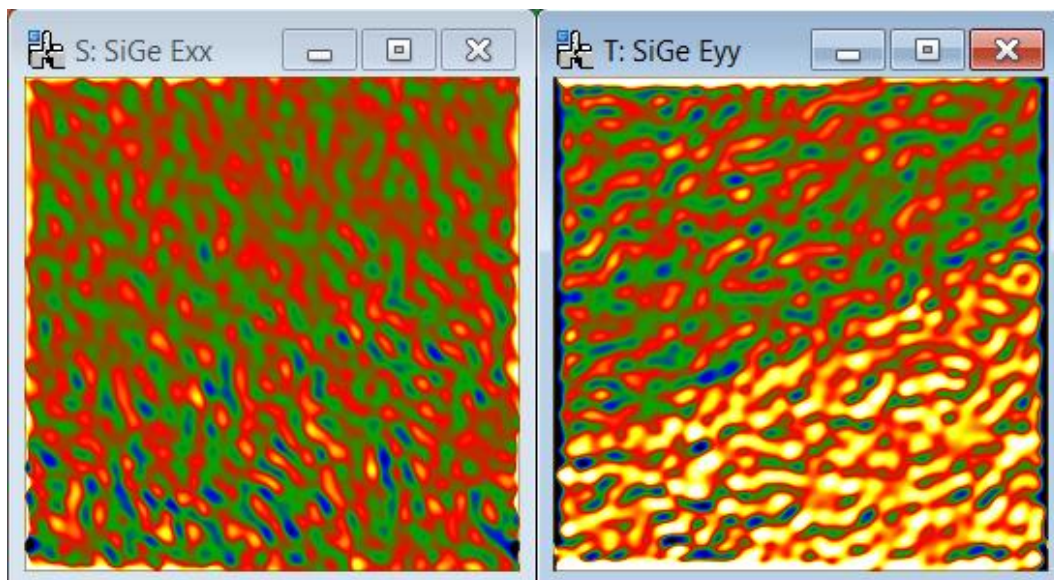

The ε_{xx} component is on average zero, indicating that the interface is coherent between the SiGe and the Si. The ε_{yy} component shows that the lattice parameter in the SiGe is larger than in the Si substrate. However, the image is rather noisy. Rather than reducing the **mask size**, let us see what using multiple phase images can do.

Recalculate the strain but this time, check all phase images as shown:
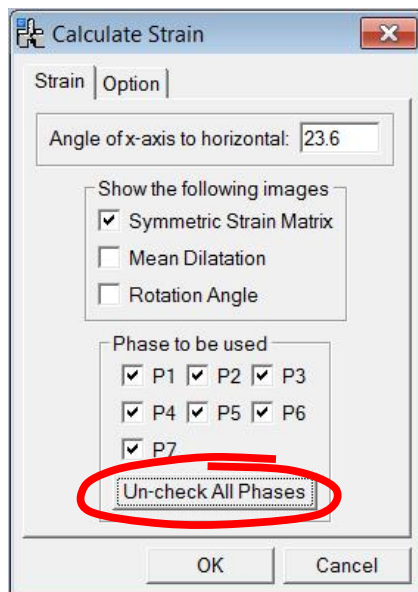
Hint: use the Check/Un-check All Phases button to select/deselect all the phase images.

All the boxes should now be ticked. You can use "Check All Phases" button at the bottom of the Phase List. Click on OK to calculate the strain map:
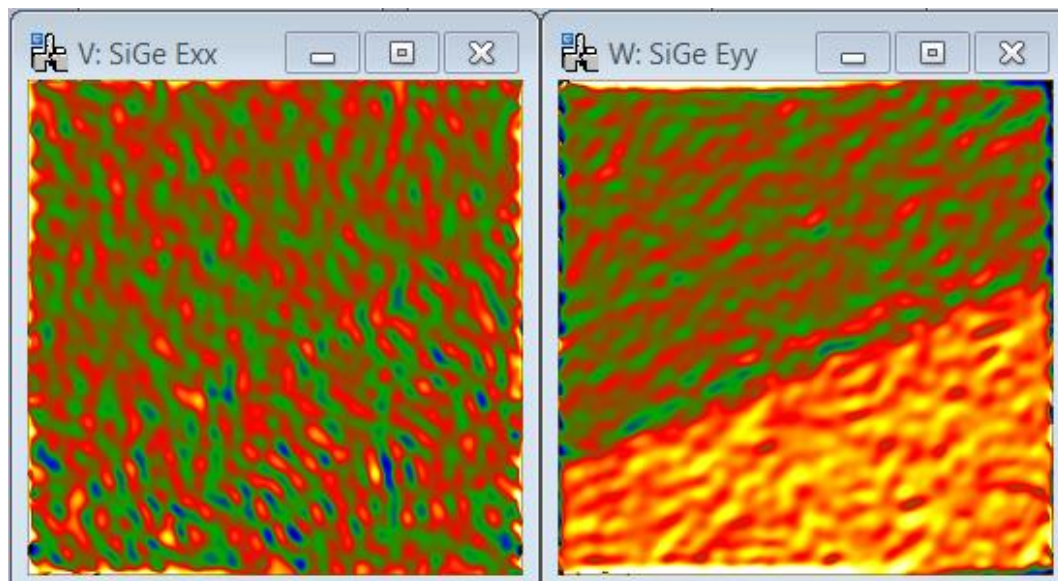
The improvement to the ε_{yy} component is impressive. What has been done? The information from all the phase images has been combined in a least-squares fitting routine to obtain the strain maps. In the default version, defined in the option menu, all the phase images are treated equally.

As always, care should be taken when interpreting the results and phase images should not be used blindly. Have a look at an alternative selection of spots:
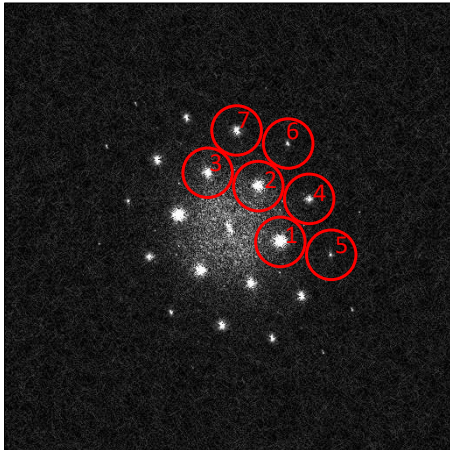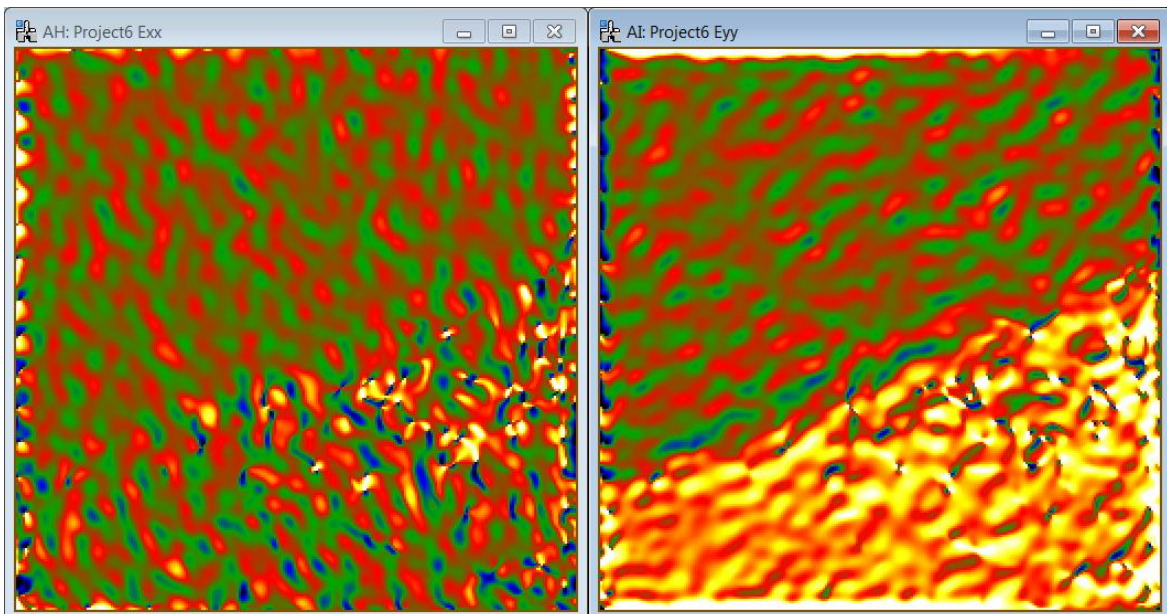
The spots 5,6 and 7 have been changed to produce the following amplitude and phase images:
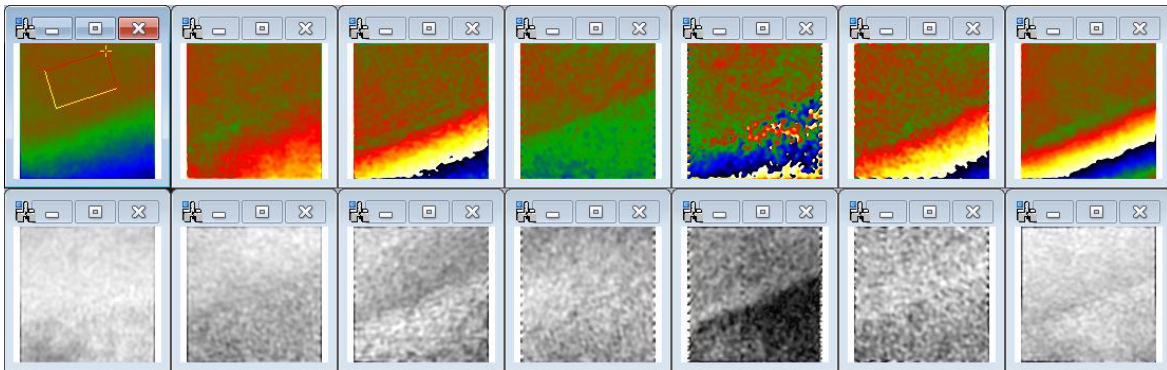
If we unthinkingly choose all the 7 phase images, the following strain maps would be obtained:

It can be seen that the strain maps are worse than with just 2 phase images! The reason can be found in the fifth phase image. The amplitude is almost zero in the SiGe layer for this set of fringes. Uncheck this phase image from the list and you will find a much better result.

As a general recommendation, look at the amplitude images and choose only phase images which you would be happy to choose when using only two phase images. Experiment, and try different spots and numbers of spots for the calculation.

Options

Not all phase images have equal significance. We have therefore included a possibility to weight the phase images in the fitting procedure, the default being no weighting (**none**). Here is the list of those options:
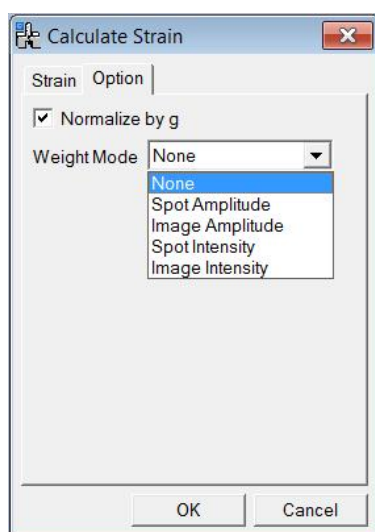
> **Hint:** choose **none** if you can after screening the amplitude images to check that all the phase images are viable.

There are different choices which you can play with: **spot amplitude** meaning the amplitude of the spot used in Fourier space (with the same weight to all the pixels), **image amplitude** meaning the corresponding amplitude image (with the weight therefore varying pixel to pixel), **spot intensity** meaning the intensity of the spot in Fourier space, and **image intensity** meaning the square of the amplitude image.

When the "Normalize by g" is checked, the weight of 1/g will be applied. This will sometimes give better result, because the phase value is proportional to g (spatial frequency), but the significances (the intensity) of the spot with high spatial frequency is normally becomes low.

Try using one of these options on the last example. You should find that the problematic fifth phase image (P5) will no longer affect the results. The resulting strain map will however have a lower signal-to-noise than the **none** option of the first set of phase images (or by deselecting P5 manually). The reason is that the spot intensities decrease rapidly and the fitting is dominated by the first 3 spots, say. As mentioned in the hint, it is always best to screen the phase images yourself before calculating the strain and use the **none** option if possible. Anyway, have fun and see what you find.

Geometric distortion correction

All optical systems distort the images they form. CCD cameras and scanners (for digitising negatives for example) introduce additional distortions. Fortunately, these geometric distortions are usually fixed for a given system. It is therefore possible to eliminate these distortions by measuring them (usually only once) and then correcting subsequent images. The procedure is described in *Hüe et al. J. Electron Microscopy 54 (2005) 181*. The paper concerns projector lens distortions but is general for all geometrical distortions. All that is necessary is an image of a perfect crystal (or any other perfectly regular lattice).

Open the image "GPA Test distortion" which is a simulation of a translation boundary:
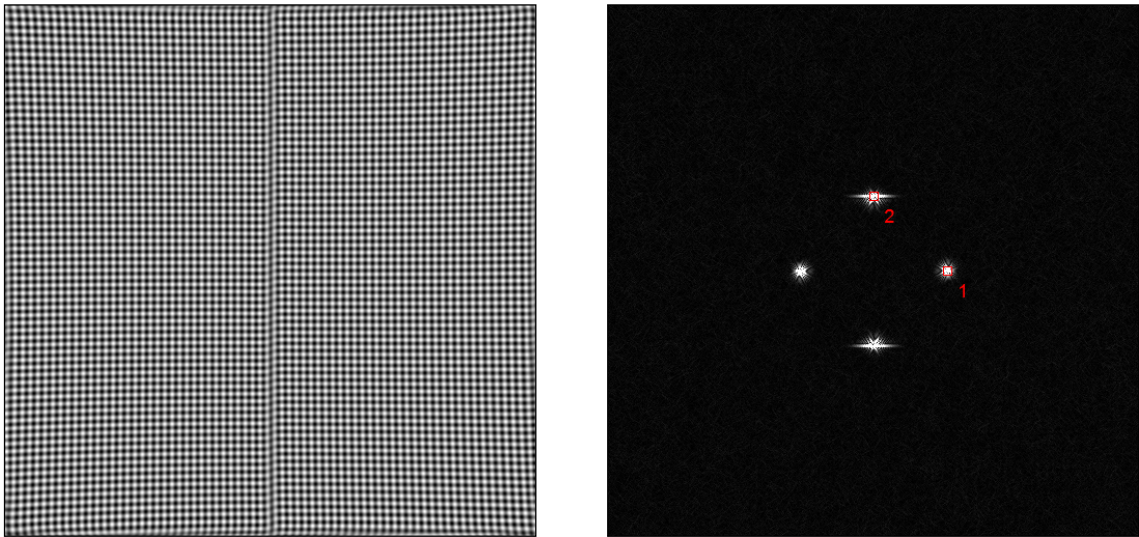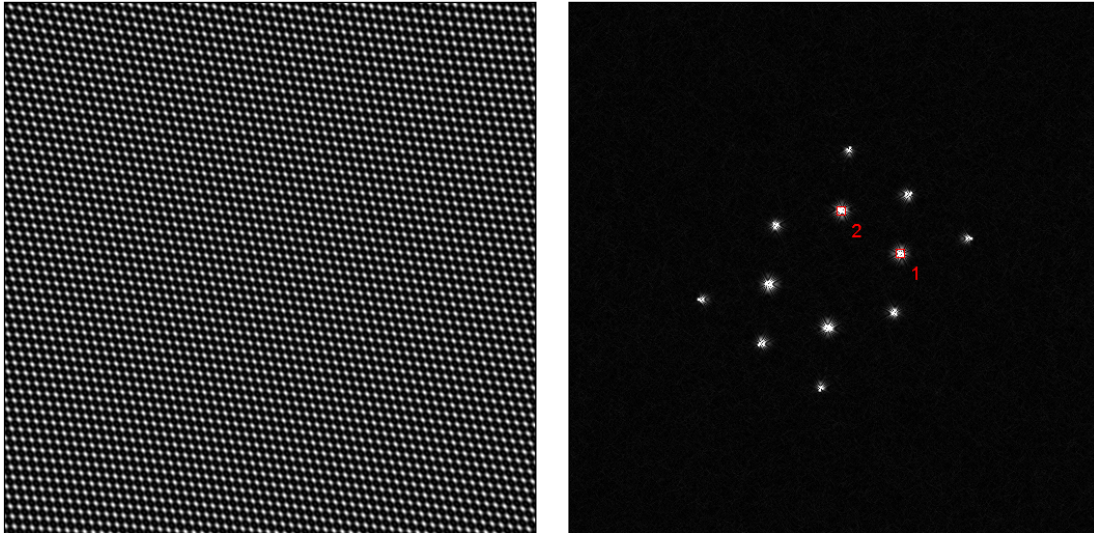

Calculate the two phase images as usual after selecting the spots in the power spectrum:
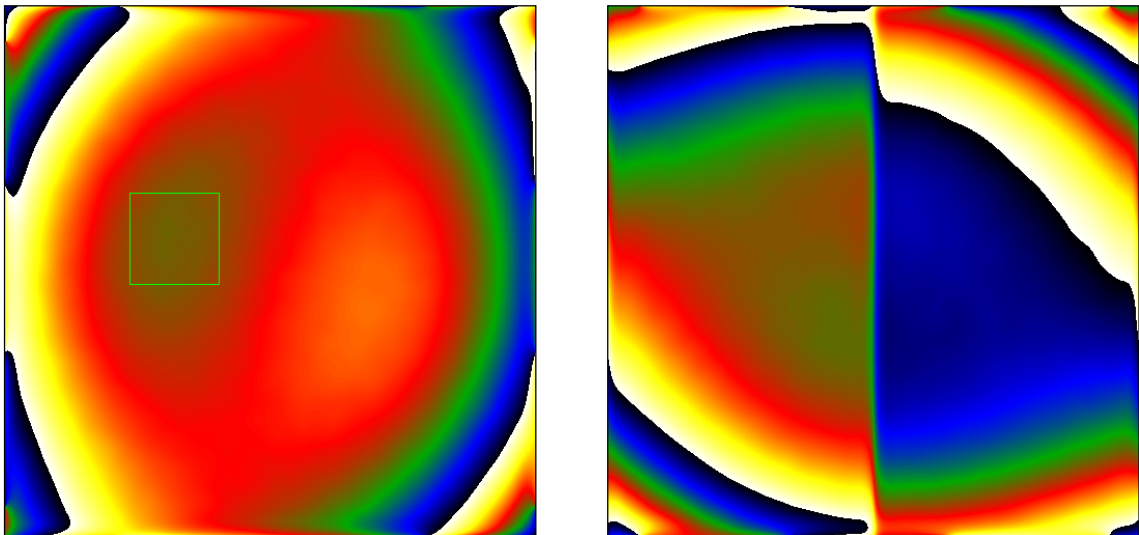
The information contained in the image is dominated by the geometrical distortions.

Distortion correction

In order to correct for distortions, you need to set up a reference image. Open the reference image "GPA Test reference" image and calculate the *Power Spectrum*.

Select two spots and calculate two phase images. In principle, any two non-colinear spots suffice.
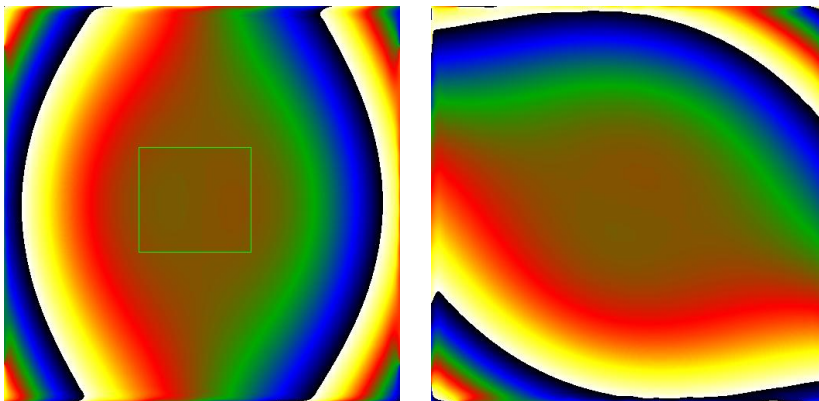
Technical note: it is not absolutely necessary to define a reference area but it is good practise.

With a phase image selected, use the menu **Distortion Info** and **Save As…** A standard Window's dialog will appear to save a file. By default, a folder is created in *My Images* folder but you can place your reference images anywhere. A good place, if you have administrator rights, is in the DigitalMicrograph folder in a folder called *GPA reference images*. Give the file a name, say "GPA Test reference", and click OK. The program will save the GPA Test reference image with the necessary information for later use.

Redo a **Phase Calculation…** for the *GPA Test distortion* image. At the menu stage, click on the **Distortion** tab. It should look something like this:
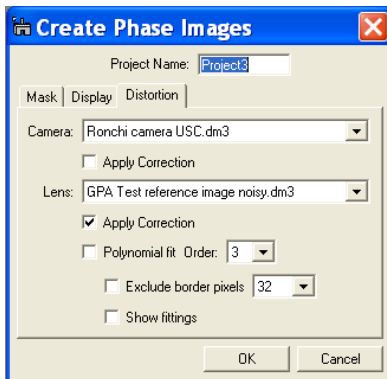
Now you can choose the reference image (Distortion Info) you want using the scroll down menu *Camera* or *Lens* depending on the type of distortion. For example, you could have a list reference images for different cameras on different microscopes. The GPA Test reference corresponds to projector lens distortions so after selecting the reference in the **Lens** menu, tick **Apply Correction** and click **OK**.

The phase images will automatically be corrected and, after using **Define Reference**, will have a nicely uniform appearance. Only the phase variation due to the crystal structure will be present:
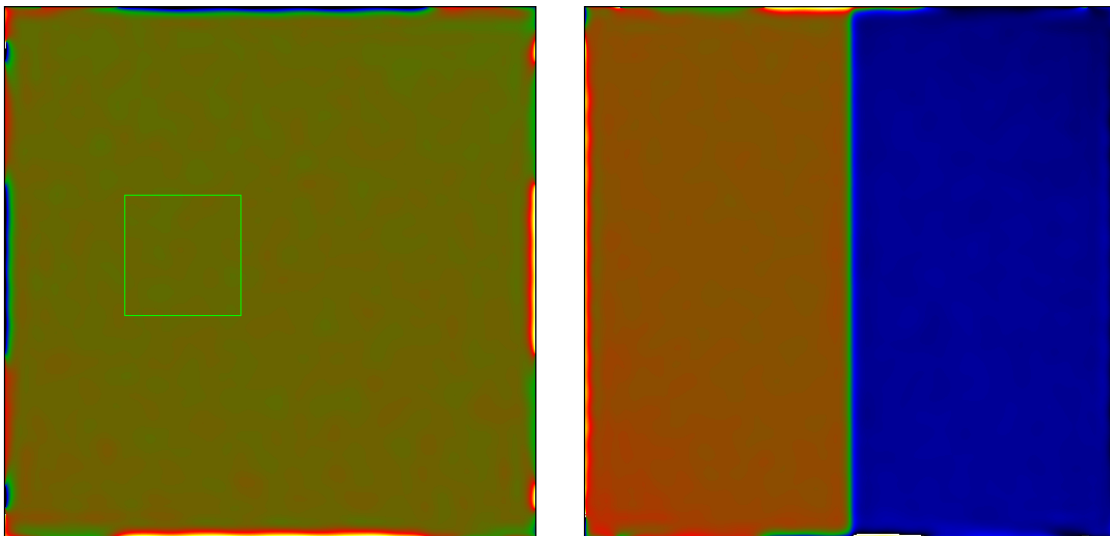
You only need to define the reference image (Distortion Info) once. From now on, it will be available in the **Phase Calculation...Distortion** tab. If you wish to delete it, just use **Distortion Info...Delete.**

Polynomial fitting

You will not always be so lucky with the reference image. Open the more realistic image *GPA Test reference noisy*:
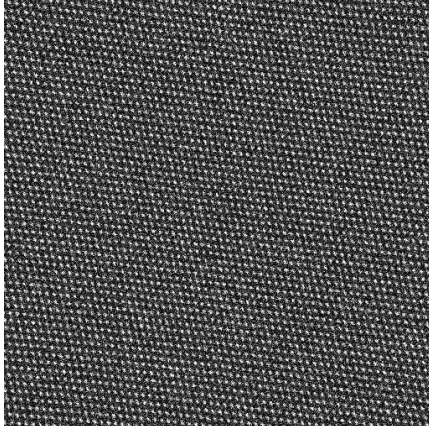
> **Technical note:** this was created simply by adding noise to the previous GPA Test reference image.

Repeat the procedure for defining a reference image for the distortions, and recalculate the phase image of *GPA Test distortion* using the new noisy reference. You will find the following results for P1 and P2:
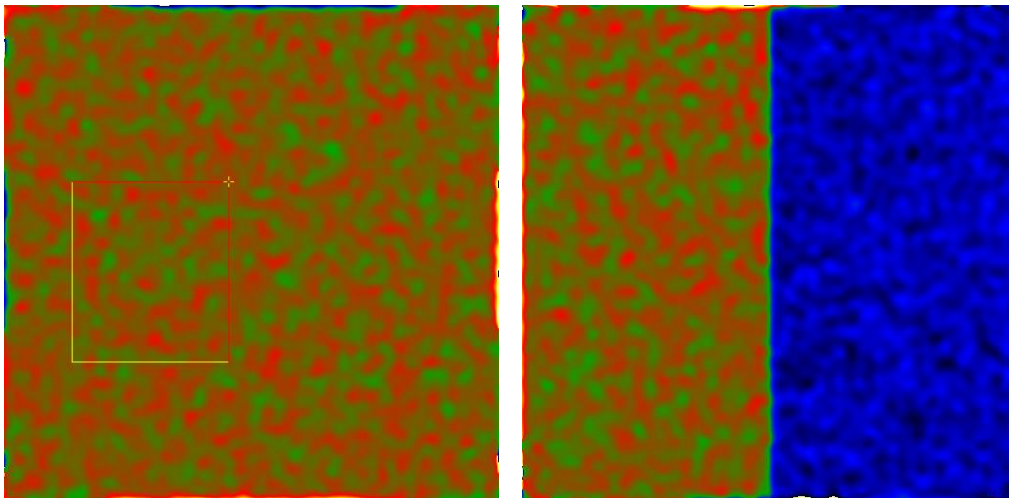
The results are much noisier than the previous example, because the noise in the reference image is effectively added to the image. To alleviate this problem, we have included in GPA Phase 3.0 the possibility of applying a polynomial fit to the reference image phases before subtracting them from the experimental phase. Recalculate the *GPA Test distortion* phases by ticking the **Polynomial fit** option:
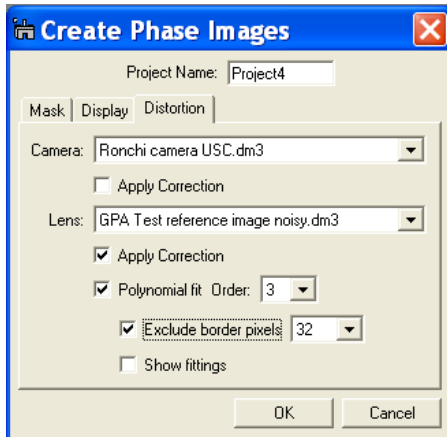
Technical note: projector lens distortions are theoretically a polynomial of order 3. It is therefore logical to use the same order for the fitting. However, higher orders can be used if necessary.

Hint: it is always worth excluding some pixels at the borders of images to avoid edge effects.

You should find the following result:
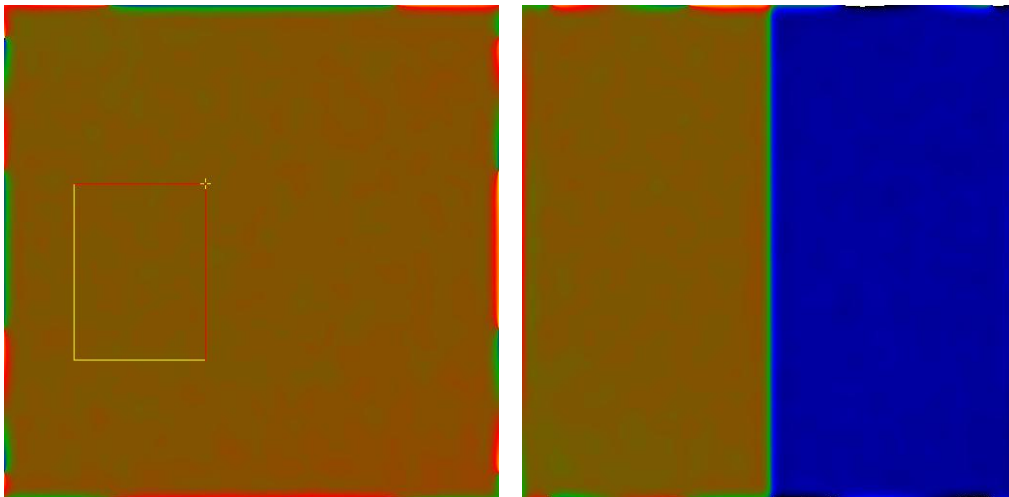
The resulting phase images are much smoother, as no additional noise has been added to the experimental phases. Indeed it would be a pity to add noise to experiments, which are already difficult to perform!

Scan-line correction (v4.5/4.12)

High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) can produce remarkable images of the atomic crystalline lattice. Here is an example from the TEAM 0.5 microscope at the NCEM Berkeley (courtesy of Marta D. Rossell). Even at 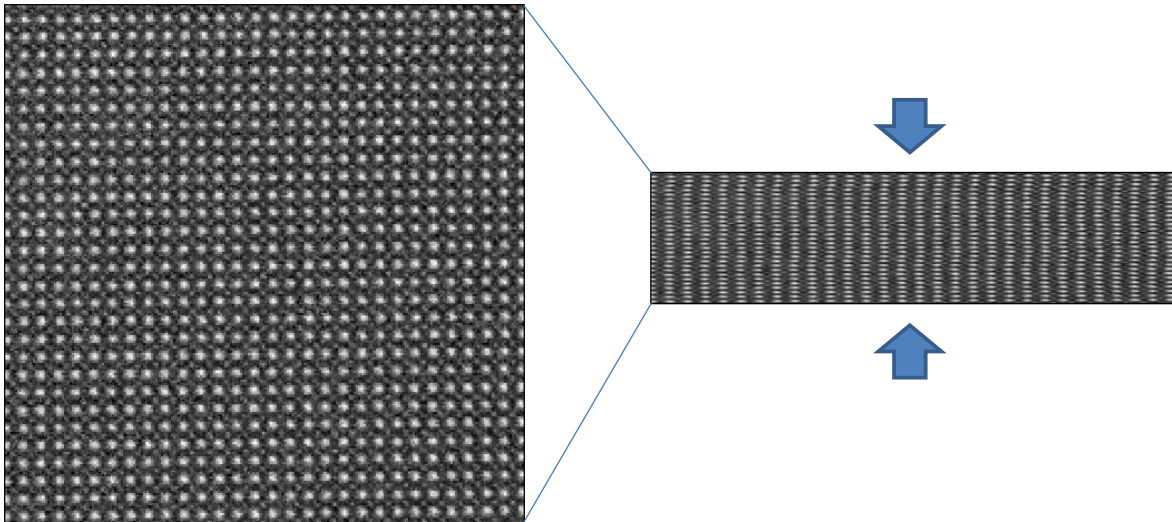relatively low magnification, the atomic columns are clearly visible and the image looks highly suitable for Geometric Phase Analysis. However, if we squash the image vertically, we can see that the atomic lattice is no longer appears straight!

This is a well-known manifestation of the scan distortion. As the beam is scanned across the specimen from left to right it can jitter, due to interference from the electronics. At the end of a line it is swept back to start a new line. However, it does not arrive in exactly the correct place. The whole line can therefore have an additional displacement with respect to the previous line of scan: the so-called "fly-back" distortion. The result is highly visible in a phase image as shown below.

Open the image "GPA scan distortion test image" which shows the full HAADF-STEM image from Marta. Calculate the phase image for the two (110) spots with a medium-sized mask.
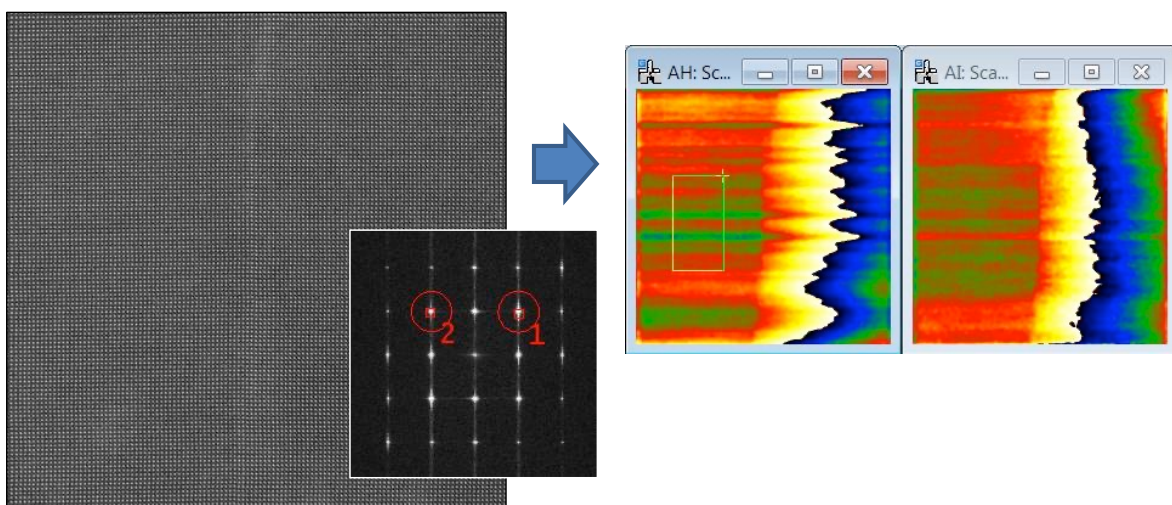
The phase images are not exactly what one would hope from a (almost) perfect crystal. However, we can see that the distortions form horizontal lines. The effect on the strain field is even more pronounced:
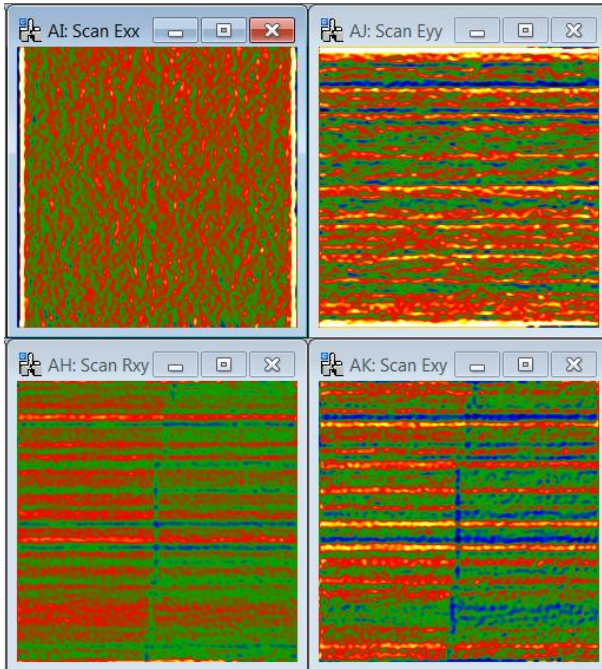
Notice that the vertical strain component, ε_{yy}, the rotation ω_{xy} and shear ε_{xy} are all contaminated by horizontal streaks whereas the ε_{xx} component is distortion free. The reason is that distortions come predominantly from the gradient of the phase images in the y-direction only.

Now let us see how the **Scan-line correction…** routines work. Here, we assume that the start point of each scan-line moves not only horizontally but also vertically due to interference from the environment.
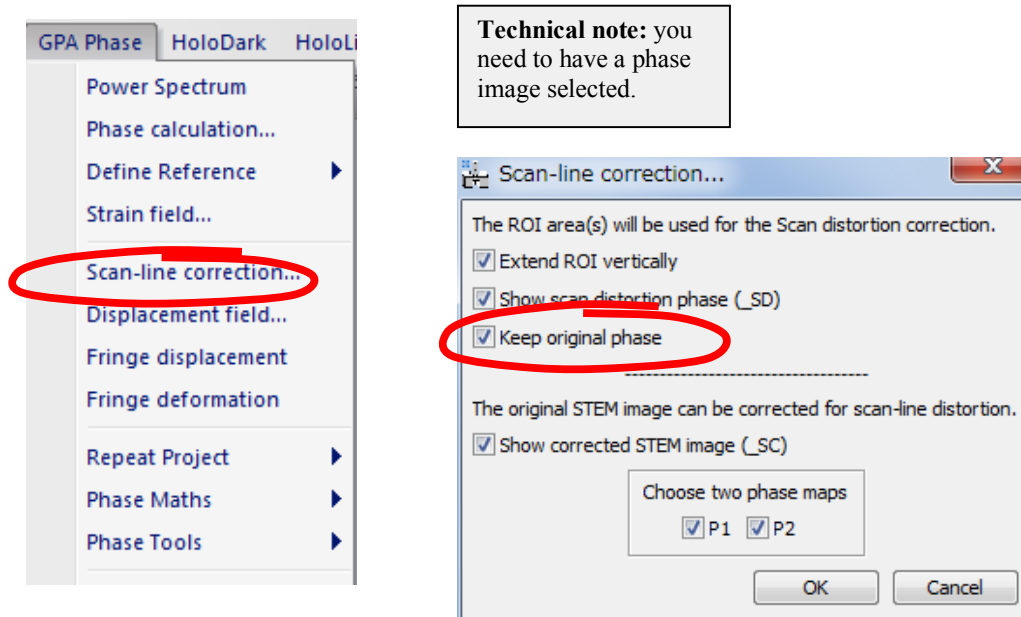
Tick the **Show scan distortion** and **Keep original phase** options so that we can follow what is happening, and you should see the following:
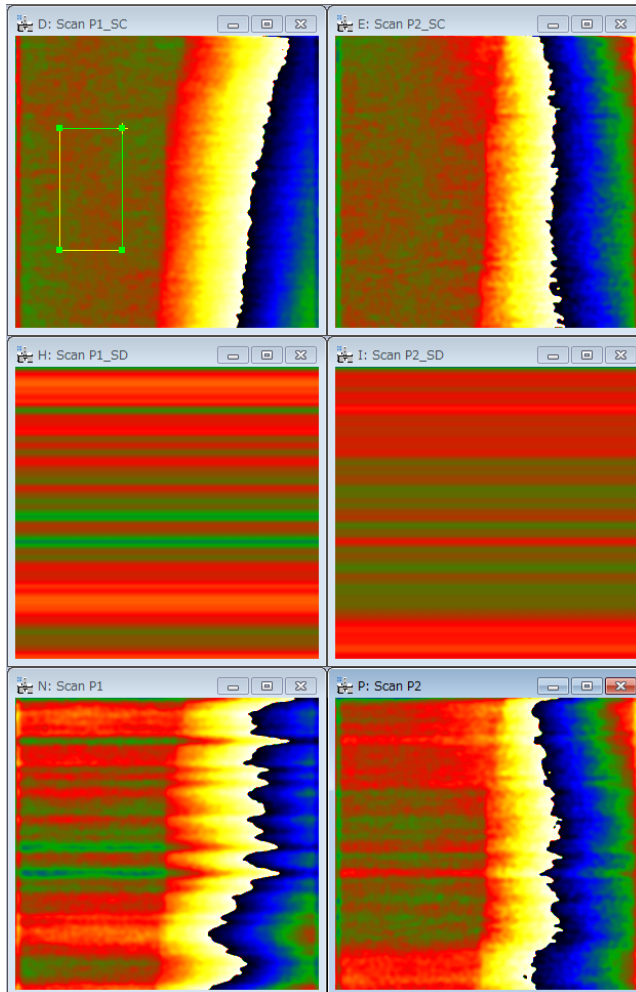
> **Warning**: the scan correction works particularly well on this example: scan nicely aligned with the lattice, relatively low magnification, and small distortions.
>
> **It will certainly not work, when there is a distortion within each scan-line!**

The phase images are now almost free of distortions. So how is it done? The routine averages the phase horizontally (along the x-direction) within a ROI for the scan distortion correction. If you want, you can use the ROI for the **Define Reference** for the scan distortion correction. The **Extend ROI vertically** option ensures that this is carried out from top to bottom of the whole image. The resulting profile is then extended horizontally over the whole image (see the phase images with _SD) and subtracted from the original phase image producing a scan-corrected phase image (denoted _SC).

These phase images give the resulting strain fields:
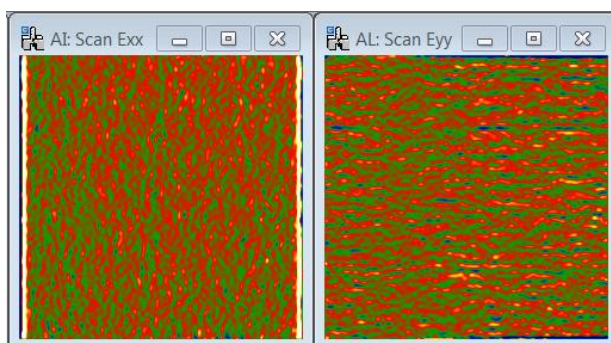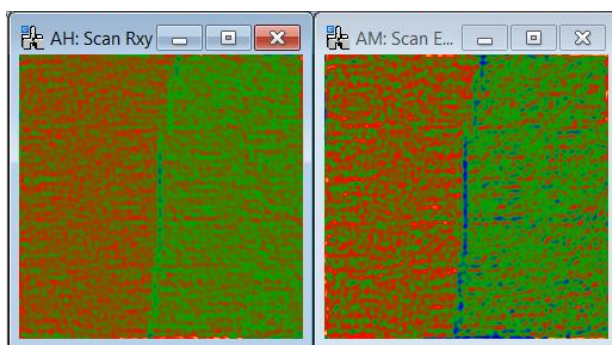
We can know see that the HAADF-STEM image was in fact taken of a twin boundary. There is neither expansion nor contraction in x and y, just a rigid-body rotation and shear of the crystalline lattice. Experiment yourself with the options to understand their effect.

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.
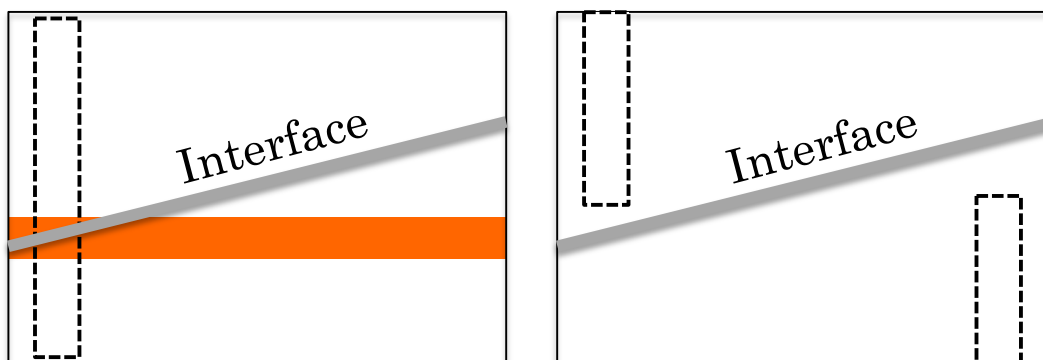
If at least two phases have been calculated without binning, the original STEM image can be corrected for the scan-line distortion. When you check "Show corrected STEM image", the STEM image corrected for the scan-line distortion will be displayed (denoted _DC).
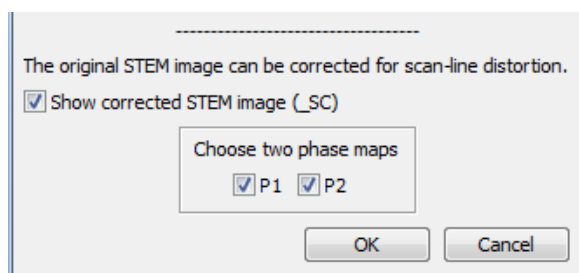
Technical note: When you calculate more than two phases, please select two of them for this command.

Scan-line corrected image

Power Spectrum of the corrected image

Difference from the original
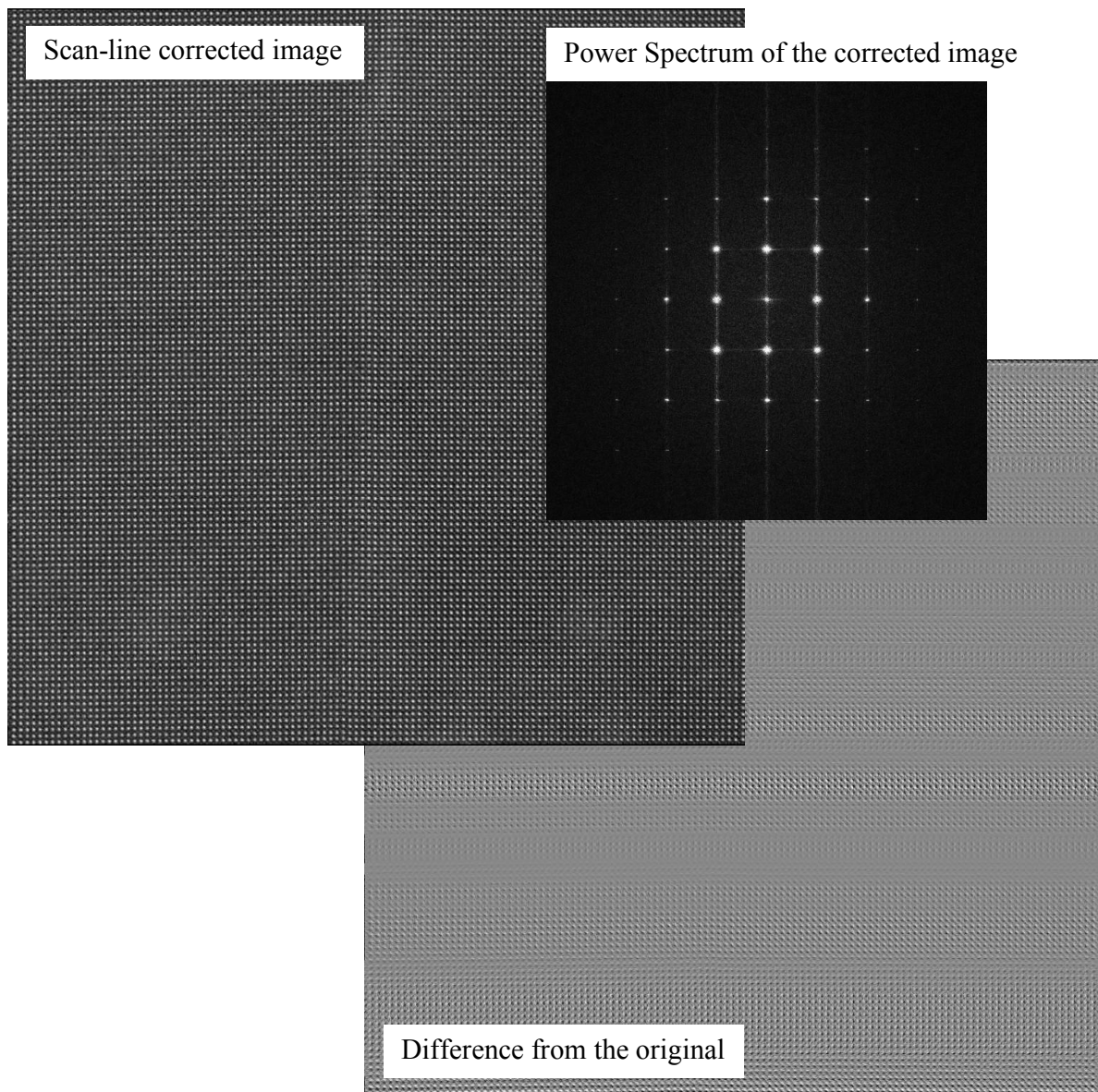
Scan-line distortion along the horizontal direction can be easily detected by eye, since the atomic lattice along the vertical direction looks wavy. Although it is difficult to detect the vertical distortion (namely, the variation of distance between the scan-lines), there should be a similar amount of distortion. The difference map above demonstrates that similar amounts of distortion appear along both directions, and the scan-line distortion can detect the distortions along both directions.

The power spectrum of the scan-line corrected image becomes sharp, which demonstrates the effectiveness of the scan-line correction.

2D vector displacements (v4.7)

We have already seen in the tutorial the command **Fringe displacements** to determine displacements in just one direction (perpendicular to a set of lattice fringes). Here, we will look at the command **Displacement field** for the determination of the 2D in-plane vector displacement field from two phase images. Open and run the script *GPA test image – 2D displacement* to create the following image and determine the Power Spectrum:
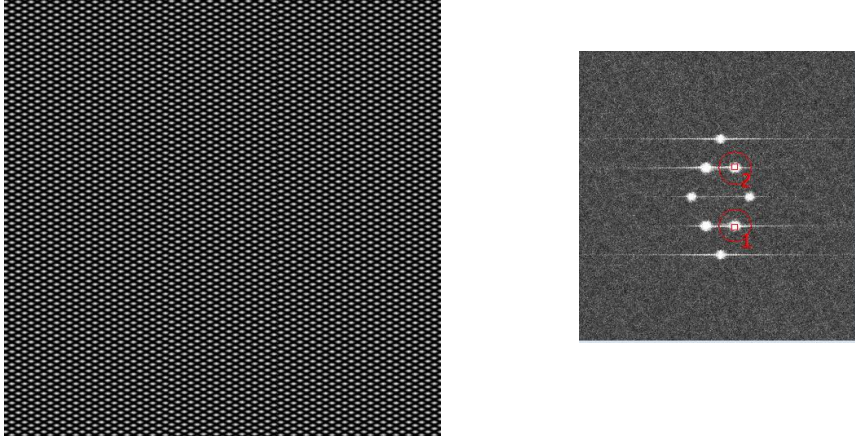
It does not look as if much is going on but calculate the phase images corresponding to the spots shown above. Define a reference region to the left and you should see the following results:
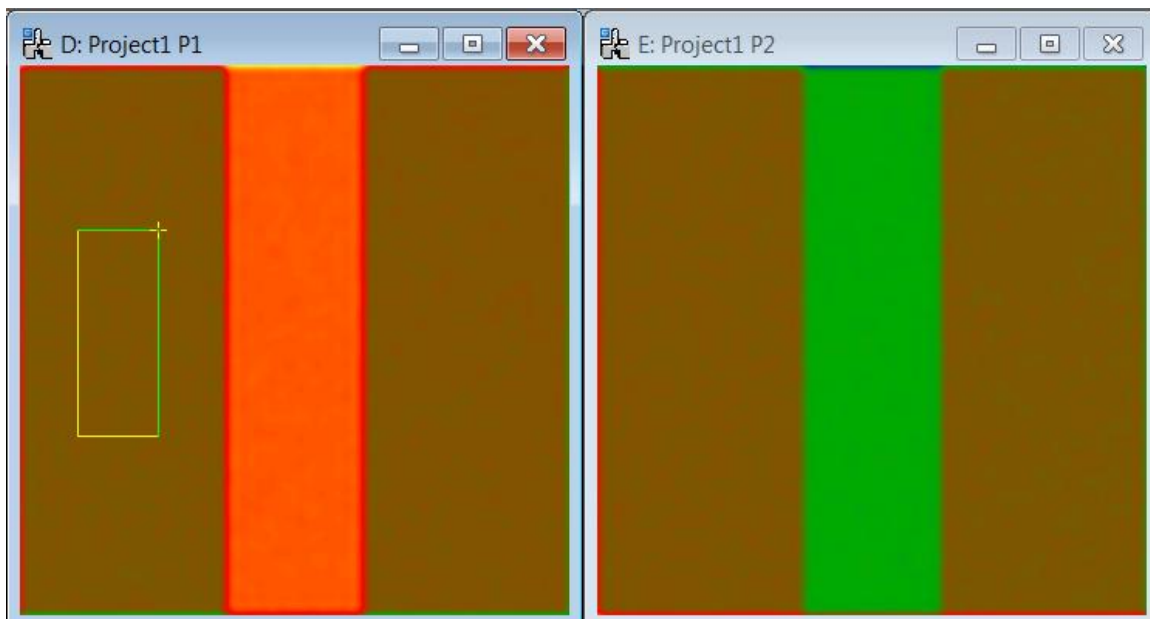
The phase images show that the central region is shifted with respect to the rest of the image. In this case, both phase image show a shift and therefore we need to combine the two phase images to determine the displacement vector (see Appendices for the equations). We can do this with the **Displacement field** command:
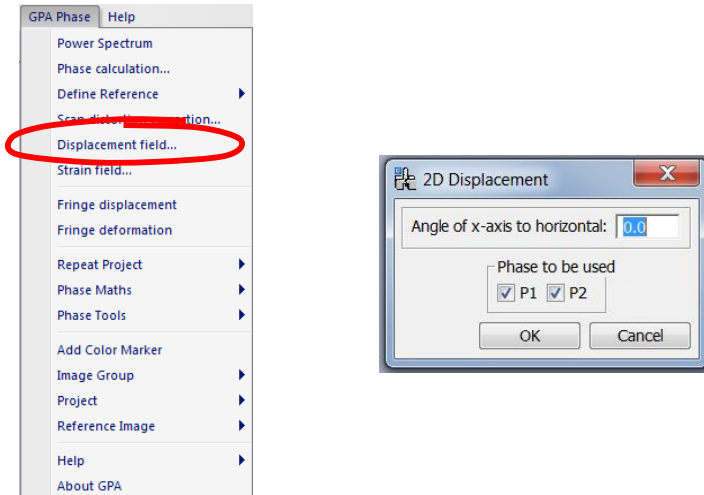
By choosing, for simplicity, the x-axis to be same as that of the image (Angle 0), the following result is obtained:
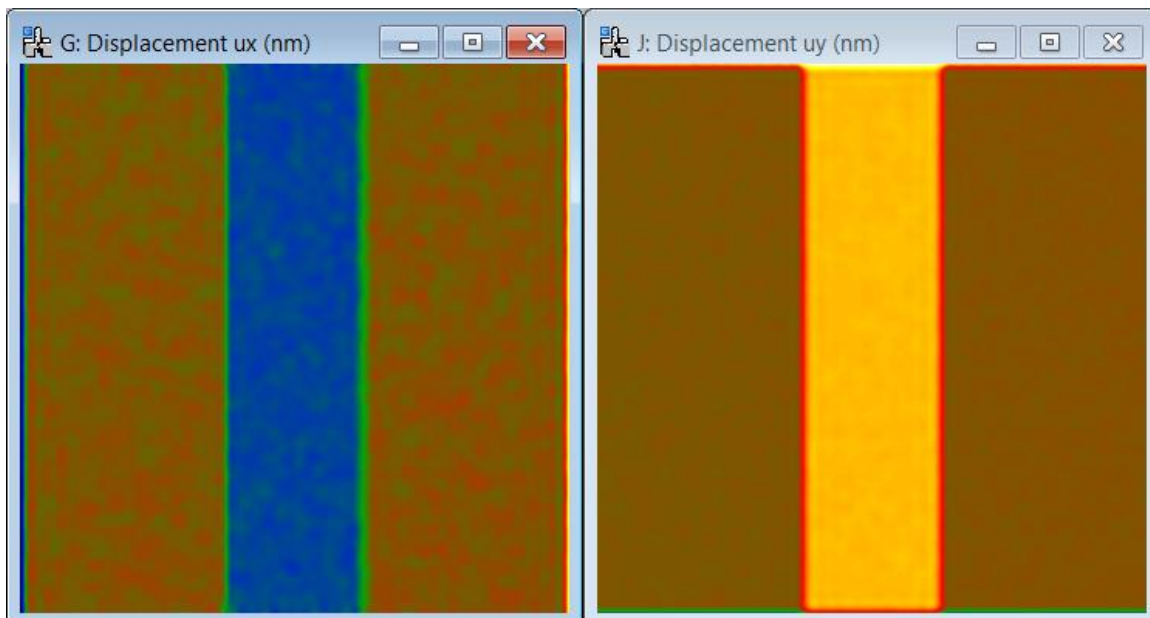
These two images represent the x and y-components of the 2D vector displacement, **u**, respectively u_x and u_y. Since the original image was calibrated in nm/pixels, the displacements are automatically given in nm.

By looking into the original script for creating the image, you can see that the central region is displaced by exactly (-0.02 nm, 0.04 nm) from the rest. Since noise has been added, the measured values will not be exactly these. Experiment with the noise level and you will see how the uncertainty is modified.

Appendixes

A: Important phase relations

Phase and displacement:

$$P_g(\mathbf{r}) = -2\pi\mathbf{g}.\mathbf{u}(\mathbf{r})$$

2D displacement and phase:

$$\mathbf{u}(\mathbf{r}) = -\frac{1}{2\pi}\left[P_{g1}(\mathbf{r})\mathbf{a}_1 + P_{g2}(\mathbf{r})\mathbf{a}_2\right] \qquad \text{where} \quad \mathbf{g}_i.\mathbf{a}_j = \delta_{ij}$$

Phase gradient and reciprocal lattice deviation :

$$\nabla P_g(\mathbf{r}) = 2\pi\Delta\mathbf{g}(\mathbf{r})$$

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 :

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

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, GPA uses the full relations suitable for large deformations (see Appendix in Hytch, Snoeck, Kilaas.)

B: Useful DigitalMicrograph commands

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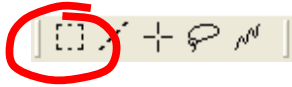
> **Hint:** to select a square area, hold down SHIFT.
> To select powers of two, hold down SHIFT-ALT.

DM **magnifying glass**:

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

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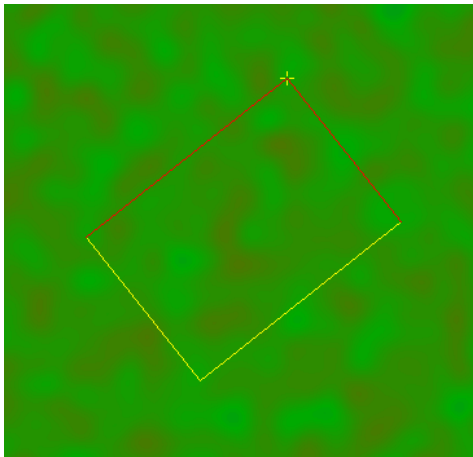
The edge length will be adjusted by one of the yellow edges, and the rotation angle will be adjusted by the yellow cross (+). (You can change the both edge lengths by dragging the yellow cross when pushing the SHIFT key.)

Quick Reference Guide

The GPA Main Menu

GPA Phase	HoloDark	HoloLi
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About GPA		
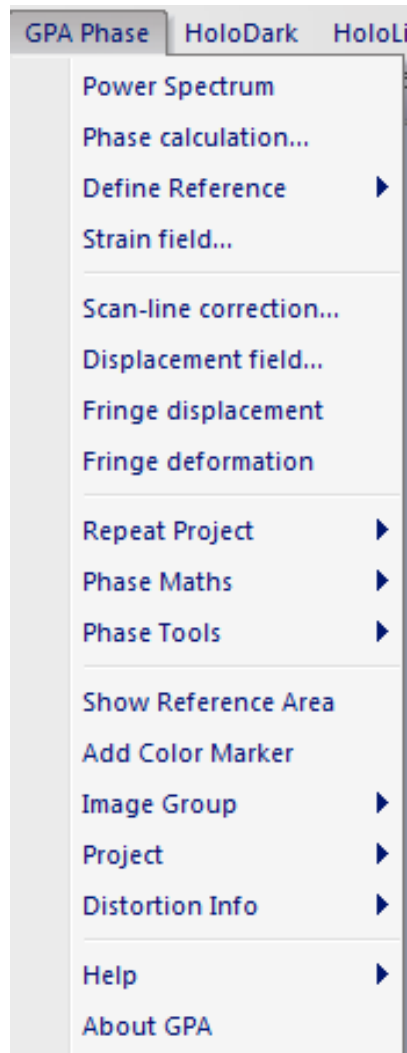
The commands in the GPA menu are described below.

Command	Description
Power Spectrum	First step in the GPA procedure. Calculates and displays the Fourier transform of the front most image. Spots are then selected in the image of the Fourier transform (called Power Spectrum) using the mouse tool.
Phase calculation…	Second step in the GPA procedure. Calculates phase images for the spots selected in the Power Spectrum. Results for each spot are displayed and managed as

|	part of a project (see options).
Define Reference (see sub menus)	Menu concerning the reference lattice and third step in the GPA procedure.
Strain field…	Calculates the two dimensional deformation tensor. Asks for two phase images and options (see below).
Scan-line correction…	Corrects scan-line ("fly-back") distortion in STEM using an average value measured within the user specified ROI.
Displacement field…	Calculates the full 2D vector displacements in the plane of the image from two phase images.
Fringe displacement	Calculates the displacements perpendicular to a *single* set of lattice fringes.
Fringe deformation	Calculates the deformation of lattice fringes from the front most phase image. Displays variation in fringe spacing (with respect to reference) and orientation (in degrees, anticlockwise positive).
Repeat Project (see sub menus)	Allows phase images and other output to be generated directly from the front most HREM image, exactly as for a previous project. Also allows details of the current project to be saved for later use (even in other sessions of DM).
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.
Show Reference Area	Show the latest reference area that was used Define Reference command. You can use this command even when the reference ROI has been deleted.
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.)
Image Group (see sub menus)	Menu to close or save groups of images within a particular project.
Project (see sub menus)	Menu to manage all the images in a particular project.
Distortion Info (see sub menus)	Menu to define Distortion Info obtained from the reference images for distortion correction due to CCD cameras or projector lenses.

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 Mask Tab below.
Display Tab	For information about the components of the Display tab, see Display Tab below.
Distortion Tab	For information about the components of the Distortion tab, see Distortion Tab 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
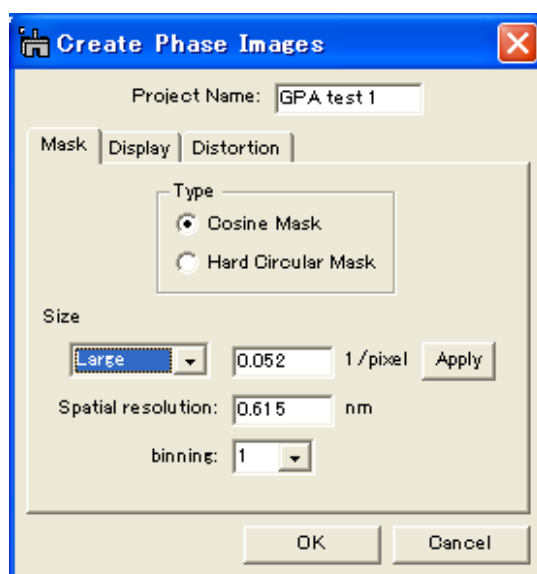
Component	Description
Type	Defines the shape of mask used to isolate the selected spots in the Fourier transform.
Cosine Mask	Half-cosine-shaped mask. Size corresponds to radius of hard cut-off and cosine quarter period (i.e. first zero).
Hard Circular Mask	Top-hat function. Size corresponds to radius of hard cut-off.
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).
Binning	Defines if the resulting phase images are to be binned with respect to the original image thus reducing their size and speeding the calculation.

Display Tab
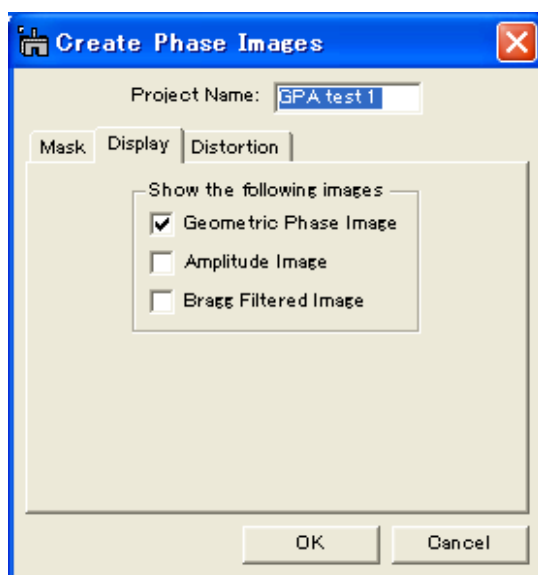
Component	Description
Show the following images	Choice of images to be calculated and displayed.
Geometric Phase Image	Geometric phase image.
Amplitude Image	Amplitude of lattice fringes.
Bragg Filtered Image	Bragg filtered image i.e. image of selected lattice fringes.

Distortion Tab
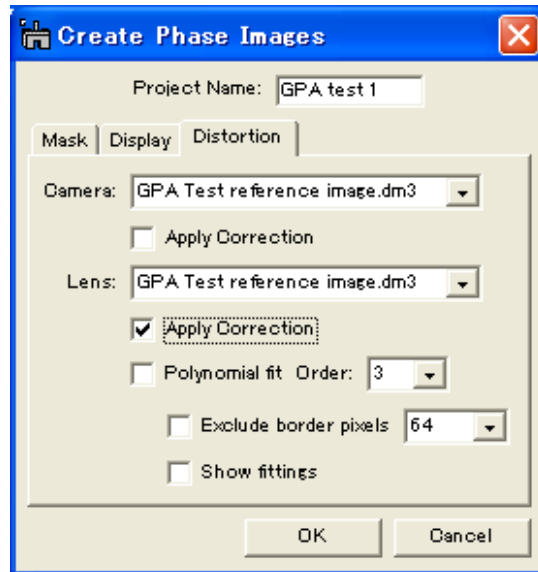
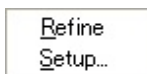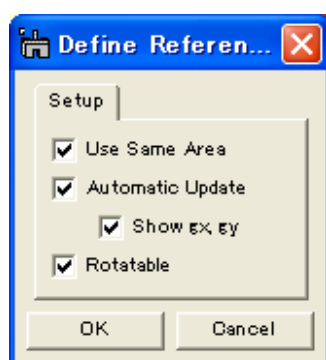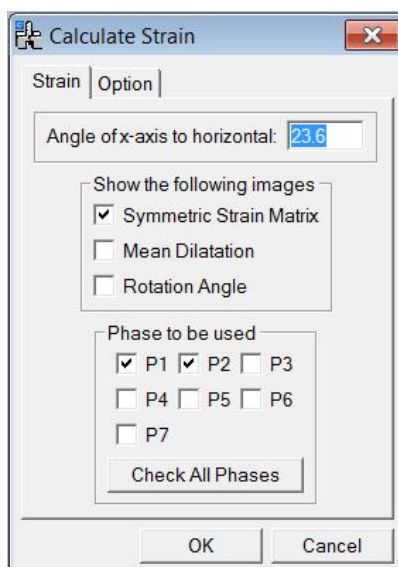| Option	Description
Camera	Selection of the distortion info obtained from reference images used for correcting camera distortions (they need to be prepared with the Distortion Info menu).
Lens	Selection of the distortion info obtained from reference images used for correcting lens distortions (They need to be prepared with the Distortion Info menu).
Apply Correction	Activates the use of the camera and/or lens distortion info to correct distortions. If both are activated, the corrections will be applied in succession.
Polynomial fit	Activates the use of polynomial fit to the lens distortion (not for camera distortion).
Order	Specifies the order of polynomial fit.
Exclude border pixels	Specifies the width of border pixels to be excluded when estimating polynomial fit parameters. (Most of the cases the border pixels are affected by discontinuity at the borders. Thus, it is a good idea to exclude some border pixels.)
Show fittings	Tick to display the polynomial fit in a new window.

Define Reference Menu

Option	Description
Refine	Third step in the GPA procedure. 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).
Setup…	Opens Setup dialog.

Setup Tab

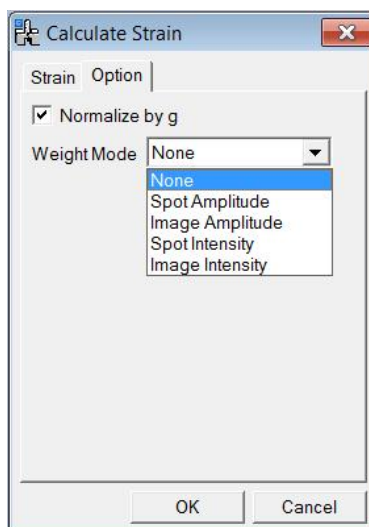| Option	Description
Use Same Area	Reference area is automatically applied to all phase images in the project when using the Refine command or Automatic Update option.
Automatic Update	Moving the reference area automatically updates the phase images and reference values.
Show gx,gy	Displays the values of the reference lattice gx and gy in the DM Results window each time the reference area is updated.
Rotatable	Tick to make the rectangular ROI rotatable. 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.)

Strain Field menu

Calculate Strain Dialog
(Strain Tab)

Component	Description
Angle of x-axis to horizontal	Defines the orientation of the x-axis used for the strain calculation. Angle defined in degrees from the horizontal plane of the image to the x-axis (anticlockwise positive). The values used for the previous calculation will be shown. ***Note***: You can specify the orientation of the x-axis by placing a Line ROI on the HREM image. In this case, the angle of the Line ROI appears here automatically.
Show the following Images	Choice of results to be displayed.
Symmetric Strain Matrix	Images of ε_{xx}, ε_{yy} and ε_{xy} to be displayed.
Mean Dilatation	Image of δ_{xy} to be displayed (average of ε_{xx} and ε_{yy}).
Rotation Angle	Image of ω_{xy} to be displayed. Values in degrees and anticlockwise positive.
Phase to be used	Select the phases to be used from the phase list.
P1 to Pn	Phase list with a check box.
Check/Un-Check All Phases	Toggle button to check/un-check all phases.

Calculate Strain Dialog
(Option Tab)

Component	Description
Normalize by g	Applies the weight proportional to 1/g.
Weight Mode	Selection from a weight list: None/Spot Amplitude/ Image Amplitude/Spot Intensity/Image Intensity.

Scan-line Correction menu

Scan Distortion Correction Dialog
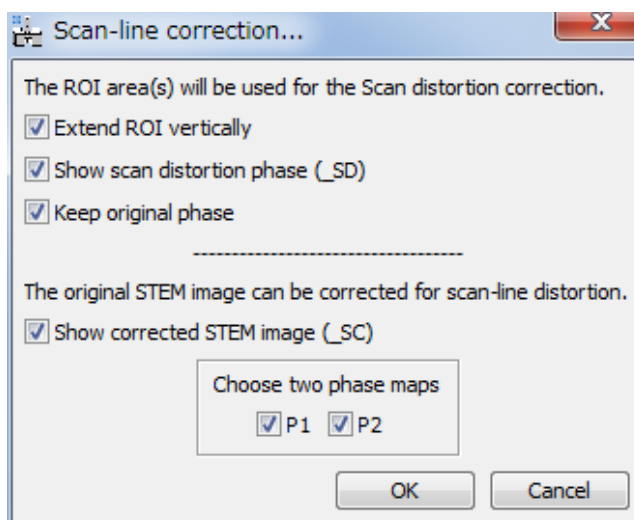
Component	Description
Extend ROI vertically	Scan distortion correction will be measured within the ROI and applied across the whole image from the top to bottom line of the ROI. If checked, the ROI is artificially extended vertically to the top and bottom of the image.

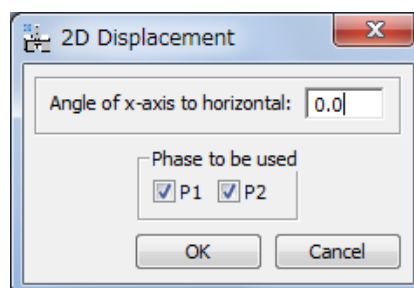|	
Show scan distortion	If checked, the phase maps (denoted "_SD") used for the scan distortion correction will be displayed. in addition to the scan-corrected phase images (denoted "_SC").
Keep original phase	If checked, the original phase images will be kept displayed.
Show corrected STEM image	If checked, the scan-line corrected STEM image will be displayed (denoted "_SC"). Here, two phase images should be selected from the phase list: P1, P2…

Displacement field menu

Displacement field Dialog

Component	Description
Angle of x-axis to horizontal	Defines the orientation of the x-axis used for the displacement field calculation. Angle defined in degrees between the x-axis and the horizontal plane of the image (anticlockwise positive). The values used for the previous calculation will be shown. Note: You can specify the orientation of the x-axis by placing a Line ROI on the HREM image. In this case, the angle of the Line ROI appears here automatically.
Phase to be used	Select *two* phases to be used from the phase list.
P1, P2…	Phase list with a check box.

Repeat Project menu

Repeat Current Project...
Repeat Saved Project...
Save Current Project As...
Clean up Project List...

Option	Description
Repeat Current Project	Repeats the same operations as carried out in the current project on the front most HREM image. Note: the current references of the phase images in the repeated project are used to calculate the new phase images. See dialog box for options.
Repeat Saved Project	Repeats the same operations as carried out in a saved project on the front most HREM image.
Save Current Project As	Saves the details of the current project for later use.
Clean up Project List	Removes project details.

Repeat Current Project dialog
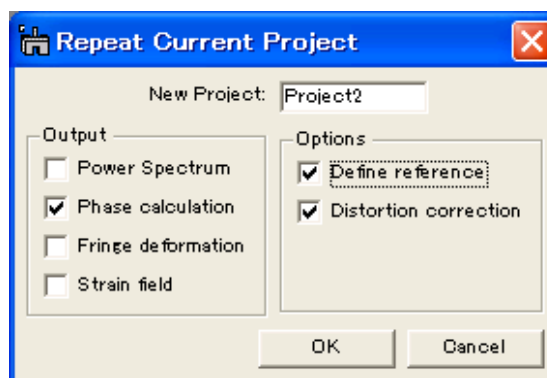
Option	Description
New Project	Defines the name of the new project.
Output	
Power Spectrum	Tick for the power spectrum to be displayed.
Phase calculation	Tick for the phase image to be displayed (including amplitude and Bragg filtered images if calculated in the repeated project).
Fringe deformation	Tick for the fringe deformation to be displayed (if calculated in the repeated project).
Strain field	Tick for the strain field to be displayed (if calculated in the repeated project).
Options	
Define reference	Tick to Define reference in the same area as for the repeated project.
Distortion correction	Tick to apply the distortion correction as for the repeated project.

Phase Maths menu

Add constant phase
Renormalise phase
Add phase images
Subtract phase images
Invert phase

Option	Description
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 phases images are in the same project, 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 phases images are in the same project, 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

Show gx, gy
Sample by 2
Contours...
Create moires
Import phase images

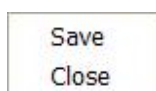| Option	Description
Show gx, gy	Displays in the DM Results window the values of the reference lattice gx and gy in 1/pixels.
Sample by 2	Rebins the front most phase image by two and multiplies the reference by two (thus preserving the reference values gx and gy in pixels^{-1} of the newly sampled image).
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.
Import phase images	Imports images into GPA, so that they are recognized as phase images. Dialog boxes will appear asking for the values gx and gy in pixels^{-1}. If the image has tags called Phase:gx and Phase:gy, these will be proposed as default. Images that are imported together will be placed in a project.

### *Contours dialog*
(Option Tab)

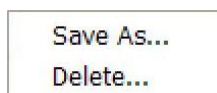| Component	Description
Contour spacing	Step in image values between each contour.
Number of contours	Total number of contours displayed.
Mid contour	Image value corresponding to mid contour.
Contour width	Contour line width in pixels.

Image Group menu

Component	Description
Save	Saves (with dialog) all images in a project of the same type as the front most image (e.g. deformation images).
Close	Closes (without saving) all images of the same type as the front most image.

Project menu
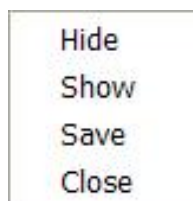
Component	Description
Hide	Hides all the images in a project.
Show	Shows all the images in a hidden project.
Save	Saves all the images in a project (with save dialog window).
Close	Closes all the images in a project without saving.

Distortion Info menu

Save As...
Delete...

Component	Description
Save As	Saves the current project image as a reference image for image distortions. Two phase images need to have been calculated. The distortion info (reference image) will then appear in the Distortion tab described in Phase Calculation.
Delete	Deletes a selected distortion info (reference image).