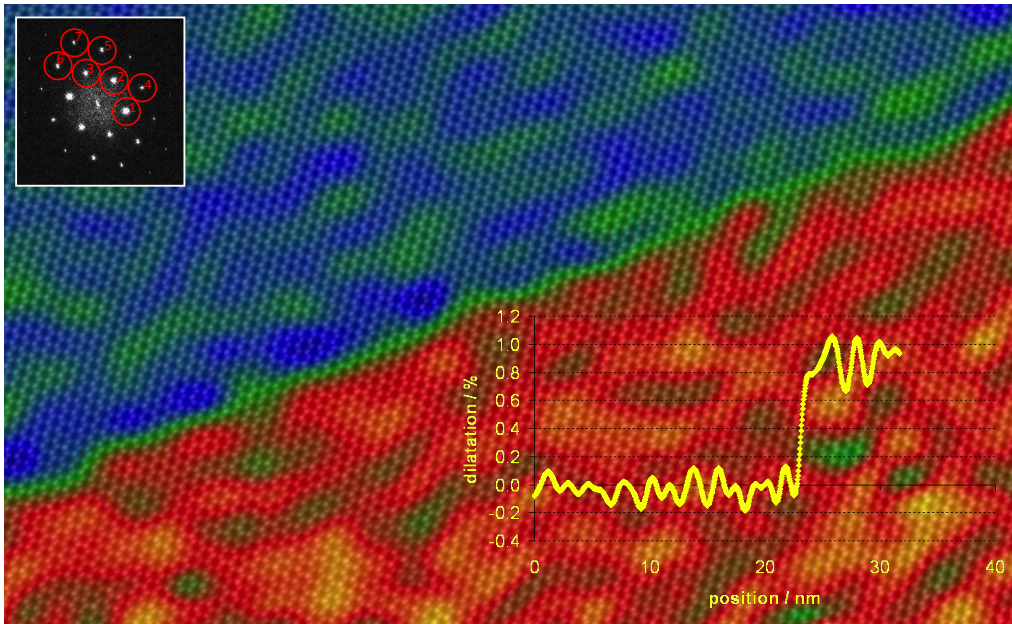


2013/01/27

GPA for DigitalMicrograph

Geometric Phase Analysis



GPA Phase Manual 4.0

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.
<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.

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Introduction to GPA

Welcome to GPA Phase the DigitalMicrograph plug-in for strain mapping from high-resolution electron microscope images, 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. Hÿe, 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](https://doi.org/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. Hÿe, 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](https://doi.org/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](https://doi.org/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](https://doi.org/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:[10.1088/0957-4416/16/10/062](https://doi.org/10.1088/0957-4416/16/10/062).
- [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](https://doi.org/10.1038/nature01638).

Software requirements

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

- DigitalMicrograph (GATAN™)
- 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.

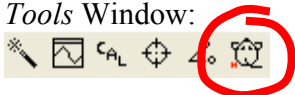
In this manual, we will dive straight into the use of the GPA Phase package with some worked examples. There is also a quick reference guide at the end of this document.

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**:



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 of version 4

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 RIO.** 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 RIO 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**

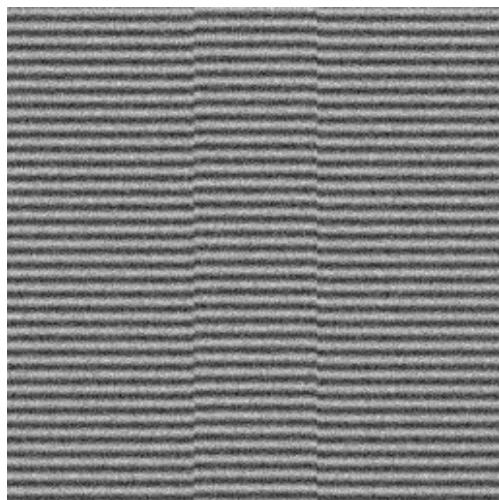
Phase...Calculate Phase. Analysing a 2048 by 2048 pixel image at binning 4 will produce results 512 square. This speeds calculations and liberates space. No information is lost, as the mask used in Fourier space is always much smaller than the original picture size.

- **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 just needs to be analysed once and saved using the new menu **GPA Phase...Reference Images**. 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

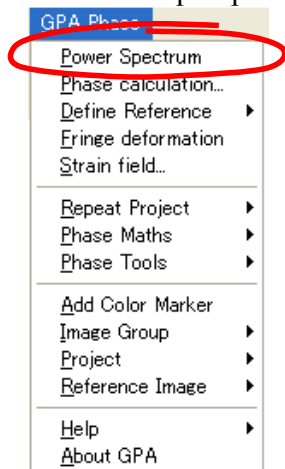
Open the image “GPA Test 0” using the DM command **File...Open** from the GPA Phase Manual folder:



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.

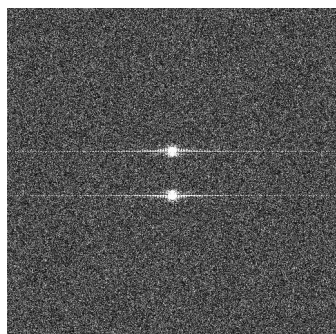
Hint: to run a script in DM, press CTRL-ENTER.

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.

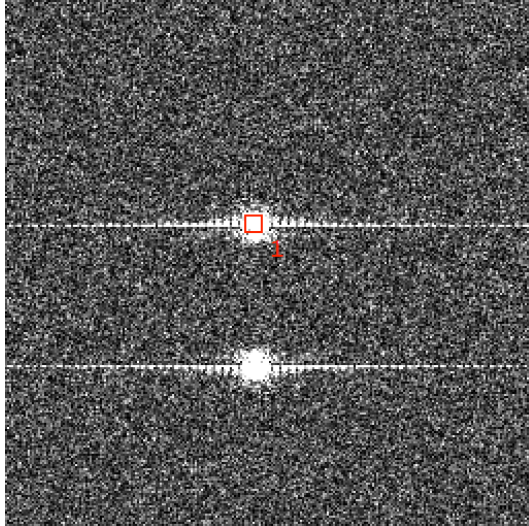
You will see an image similar to this:



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: 

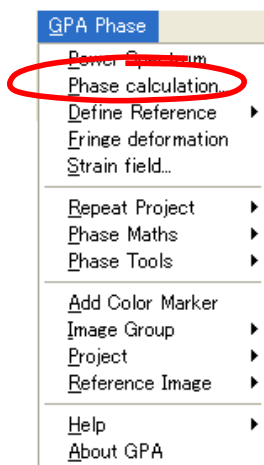


Technical note: do not worry about “hitting” the spot exactly. GPA will automatically hunt locally for the maximum intensity in the spot, even though the red square marks the actual pixel you hit.

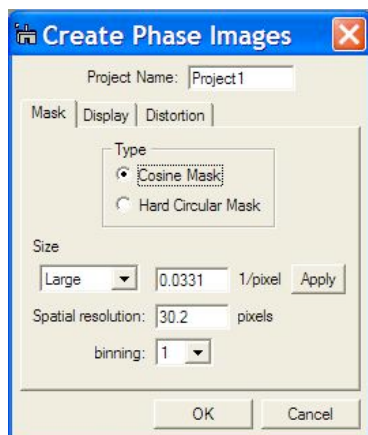
Hint: if you wish to delete your mark, click on the mouse mark again with the SHIFT key down, or use the DM **arrow tool** to select and delete.

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*:

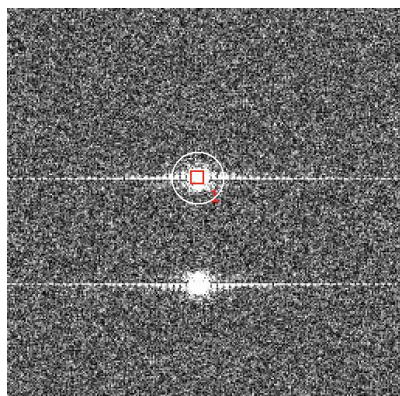


The following dialogue box will appear:



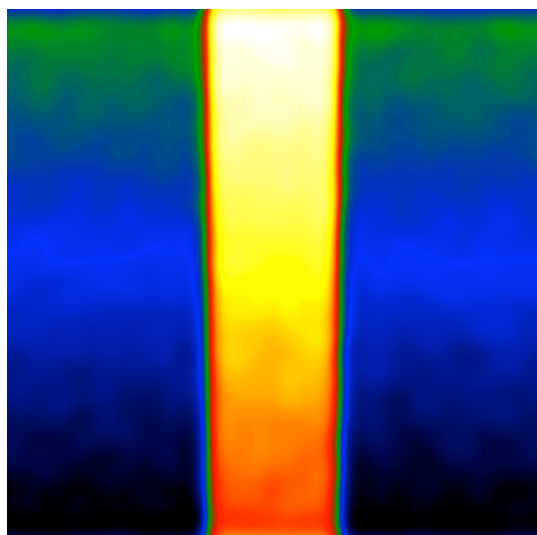
Technical note: the choice of the mask type (shape) is not that critical though the hard circular mask is to be avoided (only included for completeness). Hard masks in Fourier space introduce rippling effects in real-space, which is why smooth masks are preferred. Mask size is the most important parameter.

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*:



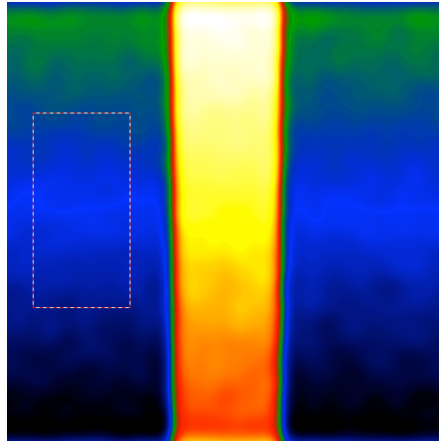
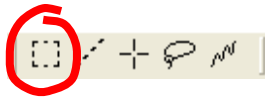
Technical note: the radius of the mask shows the area selected in Fourier space around the spot of interest. Decreasing the mask radius will produce smoother results but with less spatial resolution. The maximum recommended size is $g/2$ corresponding to the large mask size.

Now say OK and the phase image will appear:



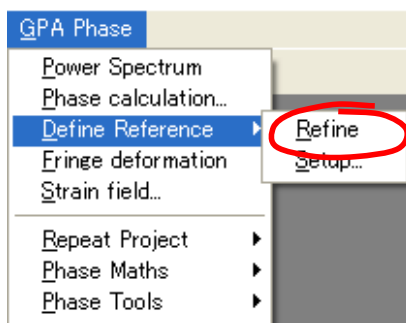
Technical note: GPA uses the temperature colour scale for displaying image values. If you prefer grey scales use the DM menu **Object...Image Display...Color**. Similarly, if you wish to change the maximum and minimum display values use DM menu **Object...Image Display...Contrast** or select an area 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 $-\pi$ to $+\pi$. 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 an area:

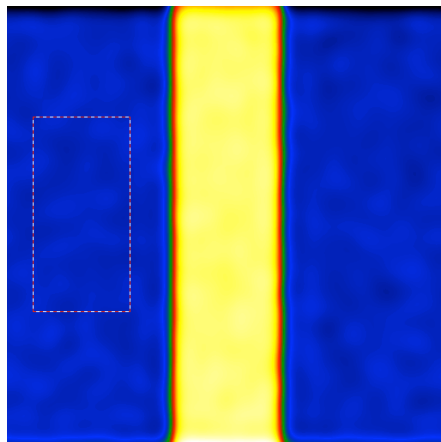


Technical note: choose an area of undistorted lattice as your reference area, recognised in the phase image as an area of uniform contrast or uniform gradient. For example, do not choose an area which straddles the interfaces. Having said that, please experiment.

and choose the next GPA phase command **Define Reference**.



The result will be the following:

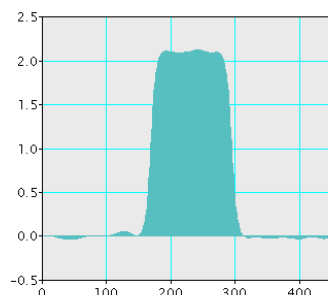
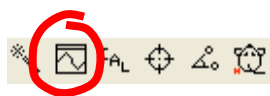


Hint: if you do not like the reference area, just grab and slide the ROI across the image. GPA will automatically update the reference area. This function can be deactivated in **Define Reference...Setup**.

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 g_x, g_y** . 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 blue). 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:

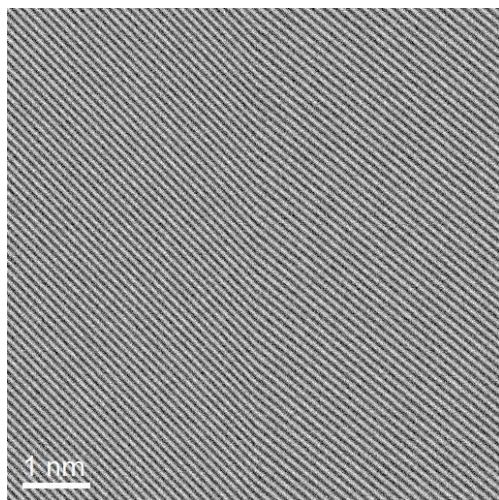


In the reference area the phase is zero and in the central band takes a value of 2.2 radians. This value can be verified in the original script used to create the image “GPA Test image 0”. From the theory, this represents a displacement of $-2.2/2\pi$ of the lattice spacing. Now choose the reference 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.

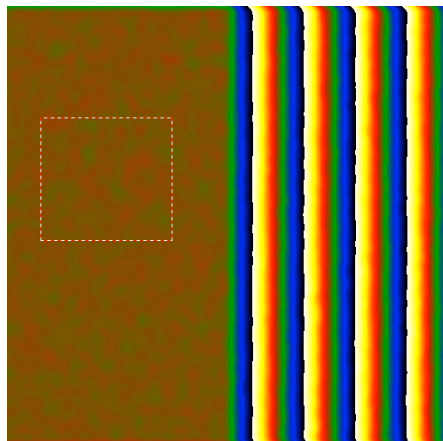
Fringe deformation mapping

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”:



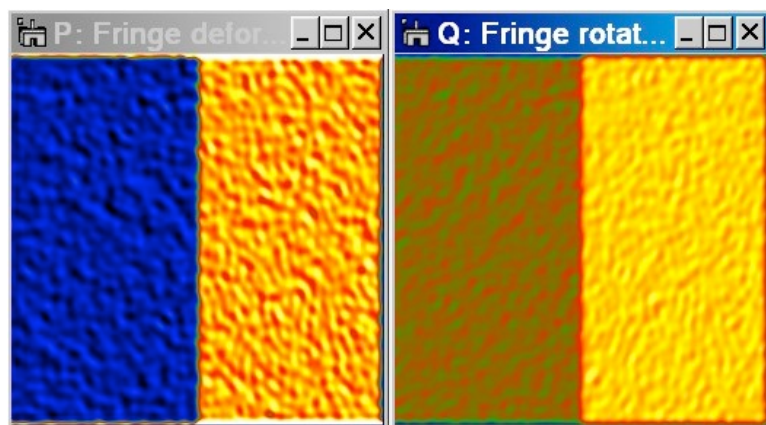
Hint: to see the lattice rotation, view the image at a glancing angle to the page. And if you like, try and measure the rotation with standard tools.

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 ($\pm 5\%$ deformation and $\pm 5^\circ$ 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.**

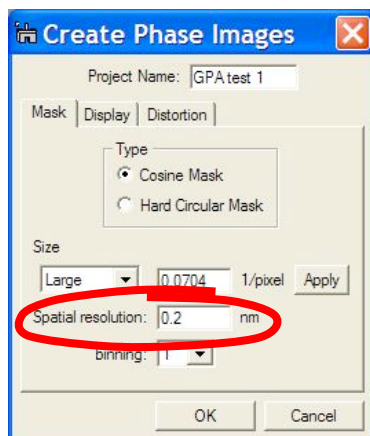
Precision and Spatial Resolution

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...

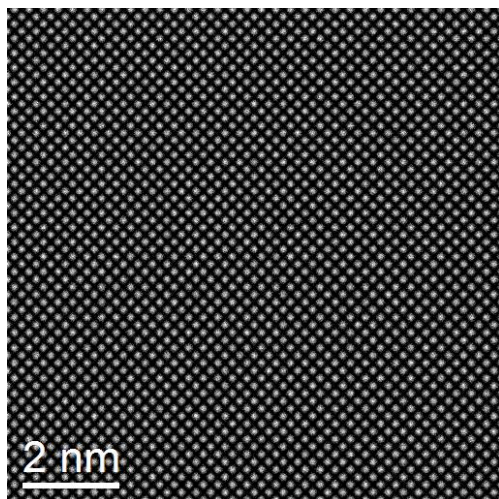
In this case, the spatial resolution of the results will be 0.2 nm. We also provide the radius of the FFT mask, κ in pixels^{-1} , which gives a spatial resolution of $1/\kappa$ in pixels. Changing the mask size will change the spatial resolution (updated automatically).

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***.

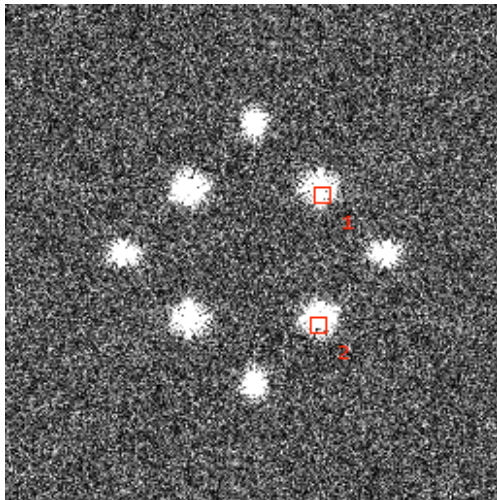
Determining strain tensors

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”:



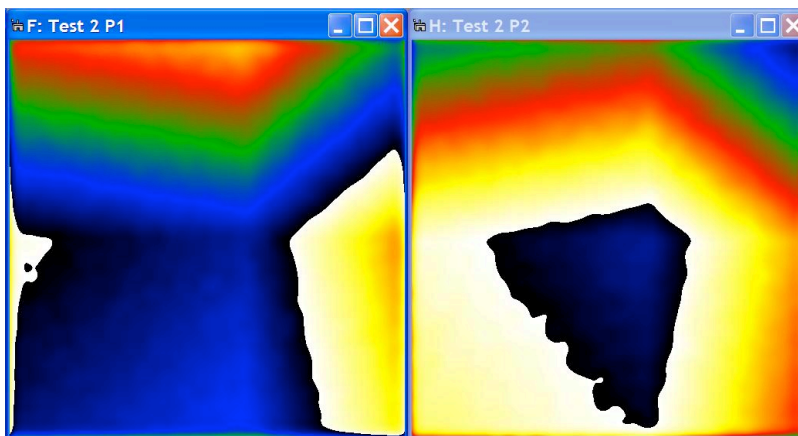
Technical note: a deformation is indeed present here, see the script “GPA Test image 2”.

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

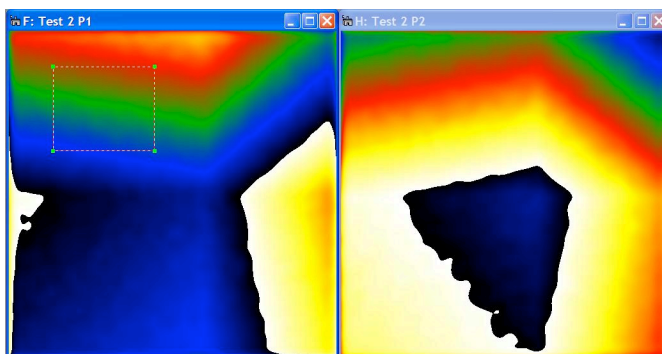


Technical note: in principle, it does not matter which two spots you choose, so long as their g-vectors are not parallel. In practice, the highest precision is obtained with low order spots and ones nearest to right-angles with respect to each other. Spots absent in the crystal structure are to be avoided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

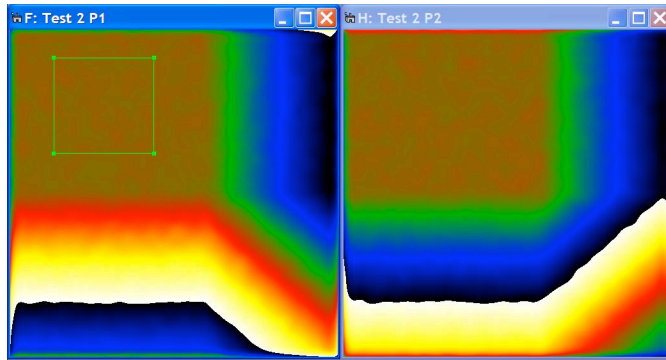


As previously, a reference lattice needs to be defined. This is done by defining an area with the **DM ROI tool** on one of the phase images exactly like the previous examples:



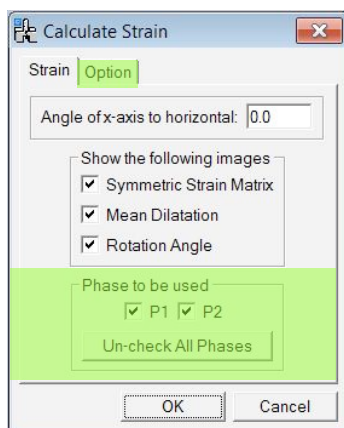
Hint: it is not always easy to recognise a good reference region. Just go ahead and try, and if necessary change the selection. Usually the situation becomes clearer after calculating the strain field.

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**.

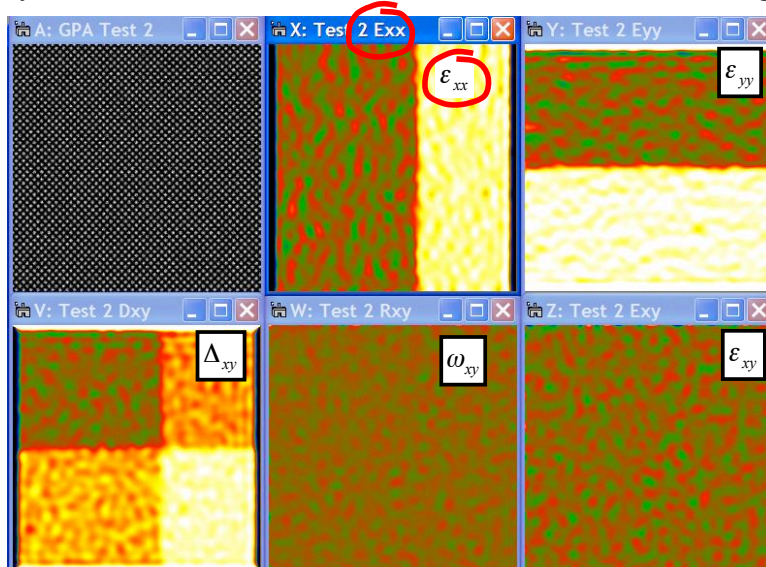
The strain tensor can now be determined with the command **Strain**. When asked, select the above two images “Test 2 P1” and “Test 2 P2” for the calculation (default values are the two most recent images). In the next dialogue, the angle requested corresponds to the direction of the *x*-axis with respect 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 $\pm 5\%$ strain and $\pm 5^\circ$ rotation.

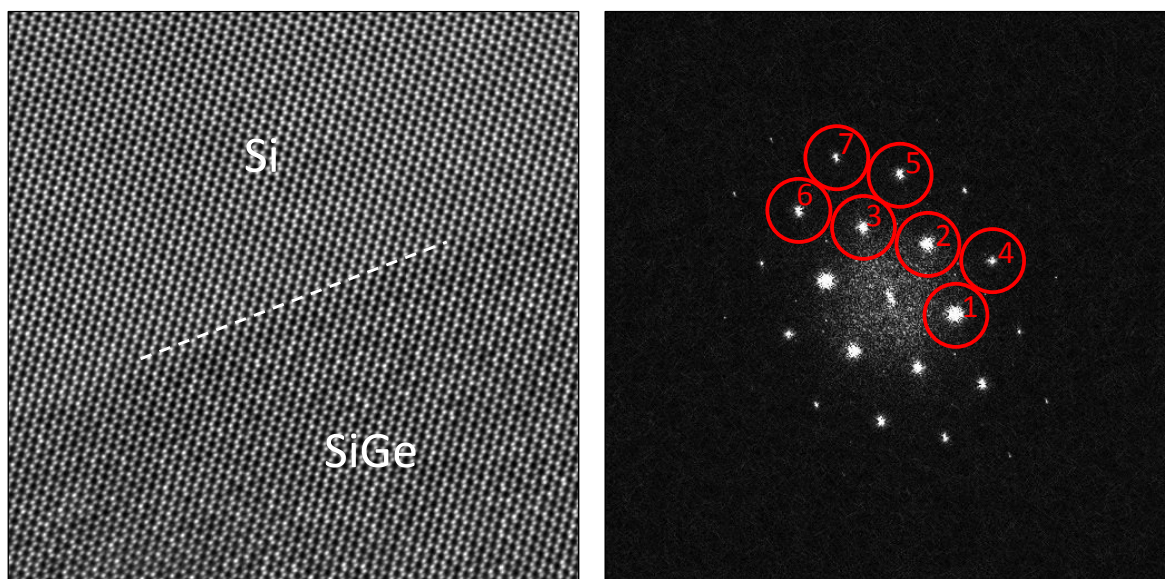
Hint: for definition of strain tensor, see the Appendix.

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!

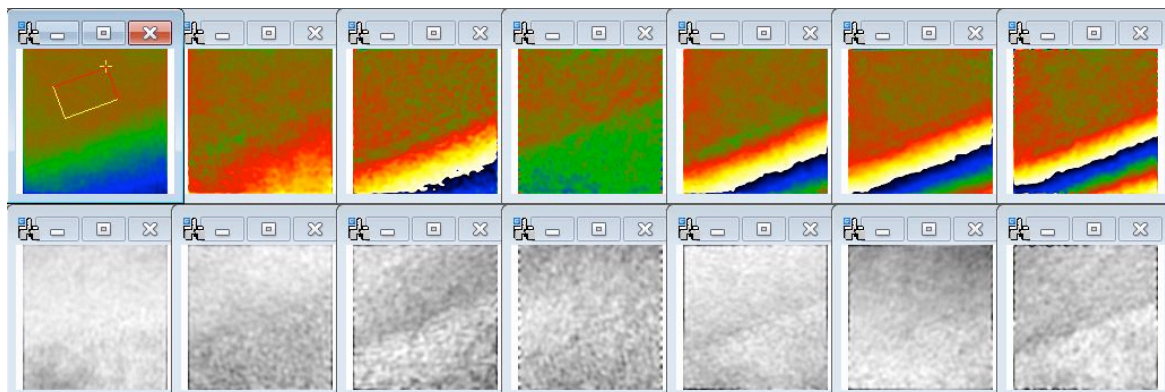
Additional functions

Strain field calculation with multiple phase images (v 4.0)

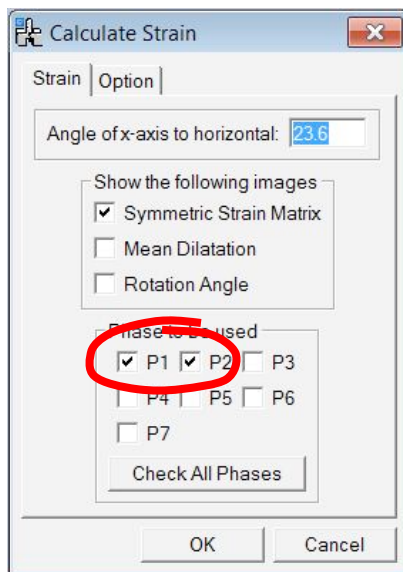
In principle, only two phase images are necessary to calculate the 2D strain tensor, and in previous versions of GPA (up to v3), strain measurements were performed by selecting the two phase images with the highest signal-to-noise ratio. However, experimental phase images are noisy, so it is maybe interesting 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:

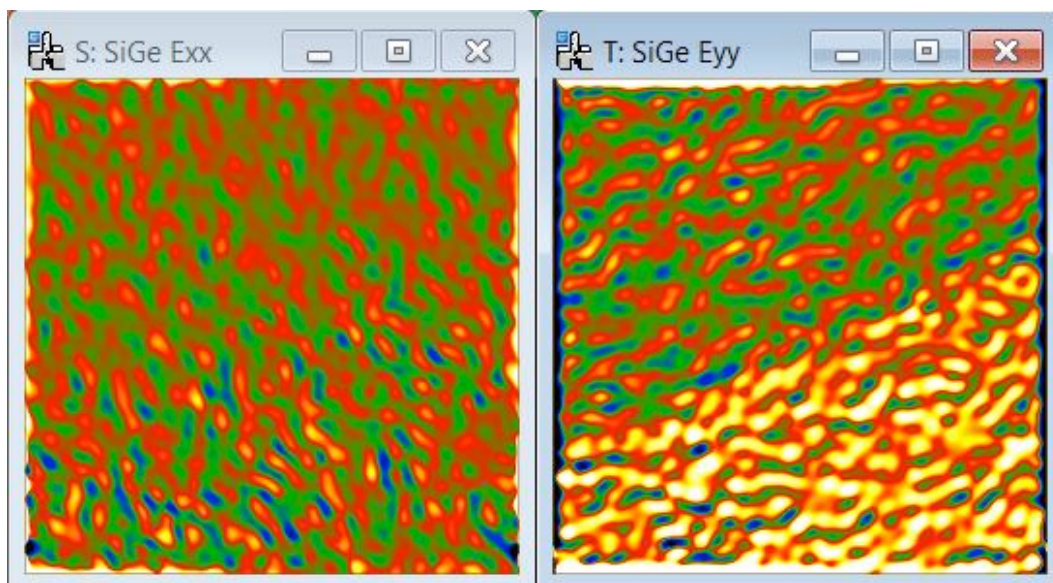


Now calculate the strain map:



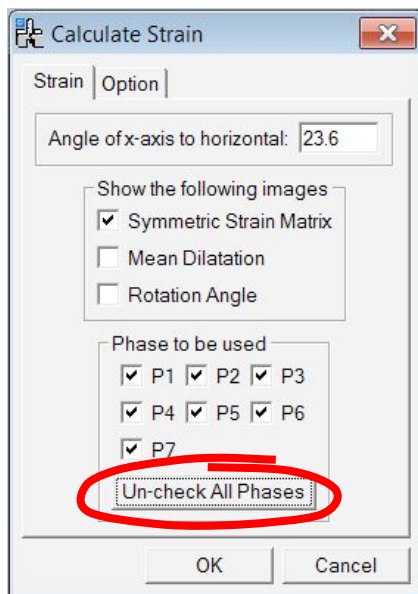
Hint: the default phase images are the two topmost phase images in DM. Check and uncheck the boxes as you like.

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:



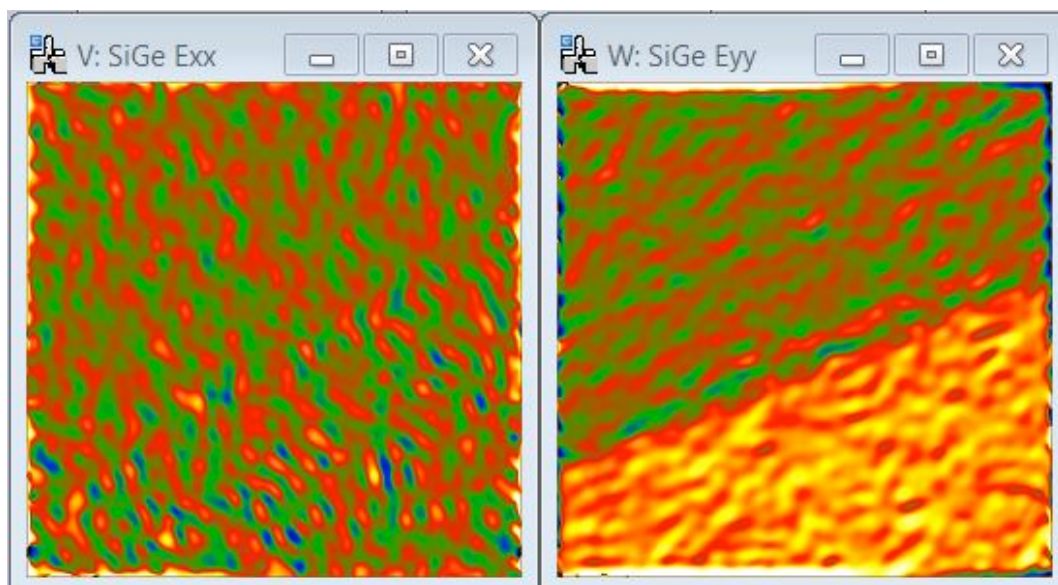
The ϵ_{xx} component is on average zero, indicating that the interface is coherent between the SiGe and the Si. The ϵ_{yy} component shows that the lattice parameter in the SiGe is larger than in the Si substrate. However, the image is rather noisy. Rather than reducing the **mask size**, let us see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

Recalculate the strain but this time, check all phase images as shown:



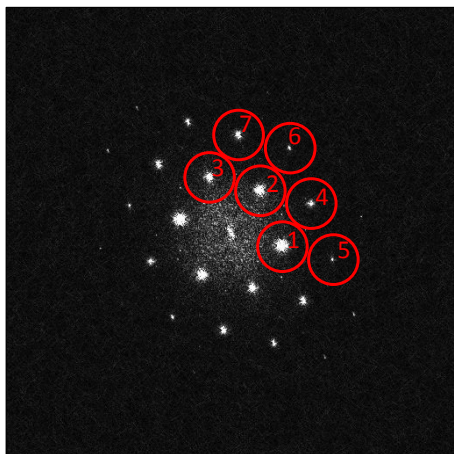
Hint: use the Check/Un-check All Phases button to select/deselect all the phase images.

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:



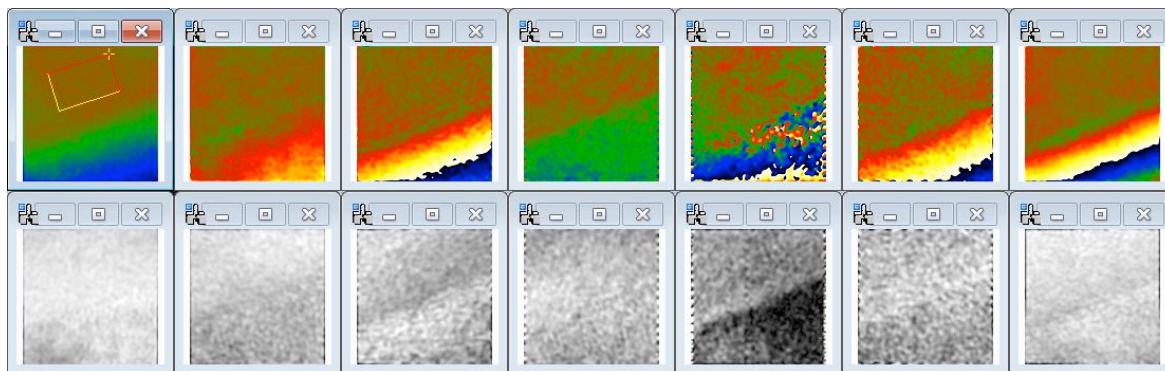
The improvement to the ϵ_{yy} component is impressive. What has been done? The information from all the phase images has been combined in a least-squares fitting routine to obtain the strain maps. In the default version, defined in the option menu, all the phase images are treated equally.

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:

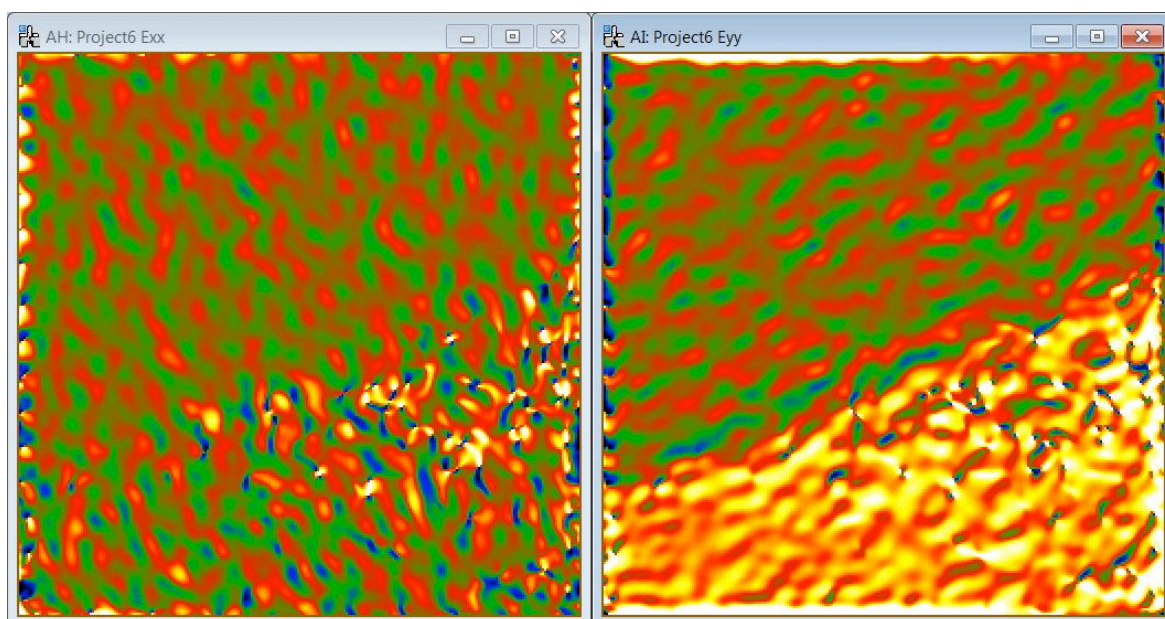


Hint: remember to unselect spots with the **mouse tool**, just hold down SHIFT and click on the spot to delete.
In this case, unselect the old spots 5, 6 and 7, and select new 5, 6 and 7 spots as shown.

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:

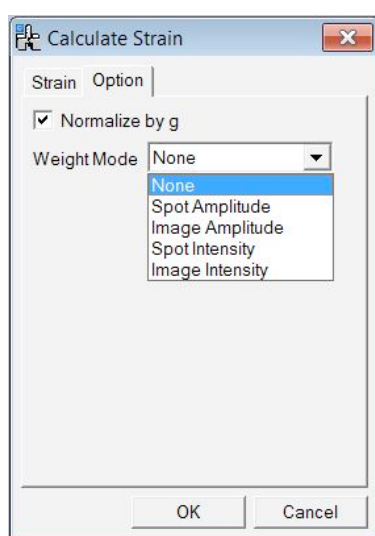


It can be seen that the strain maps are worse than with just 2 phase images! The reason can be found in the fifth phase image. The amplitude is almost zero in the SiGe layer for this set of fringes. Uncheck this phase image from the list and you will find a much better result.

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.

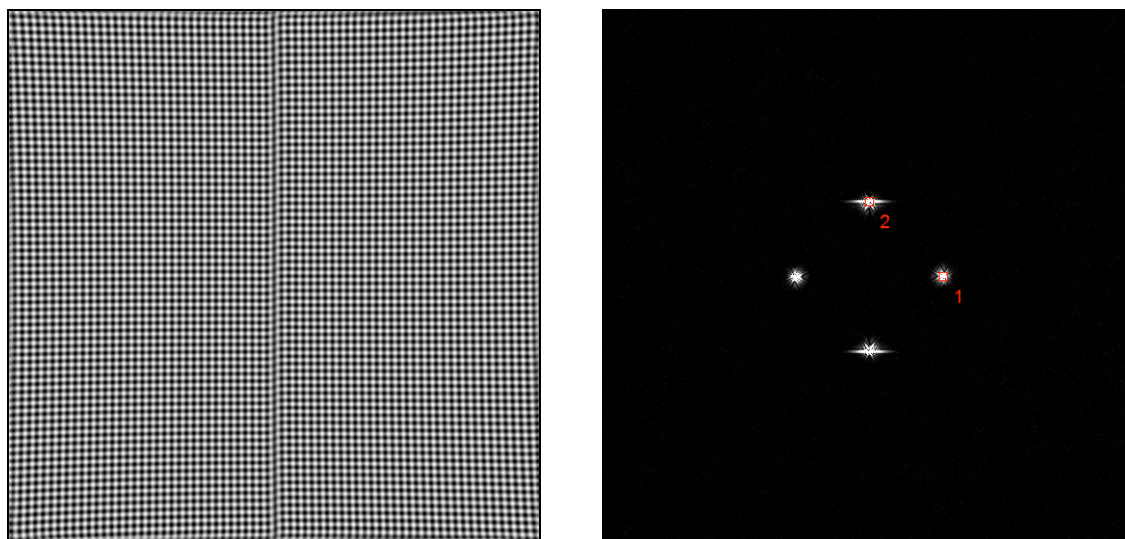
When the “Normalize by g” is checked, the weight of $1/g$ will be applied. This will sometimes give better result, because the phase value is proportional to g (spatial frequency), but the significances (the intensity) of the spot with high spatial frequency is normally becomes low.

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.

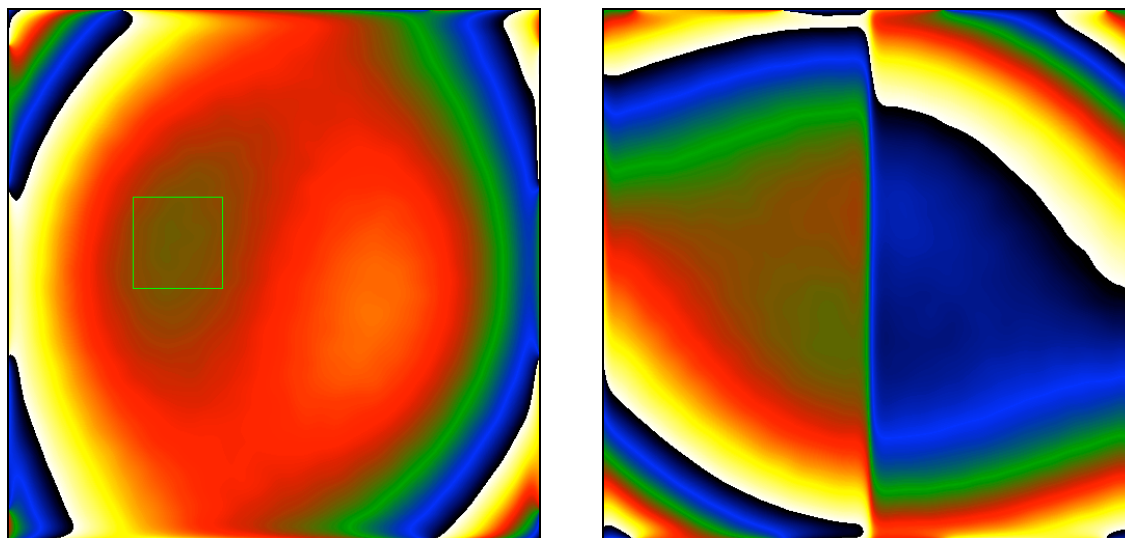
Geometric distortion correction

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:



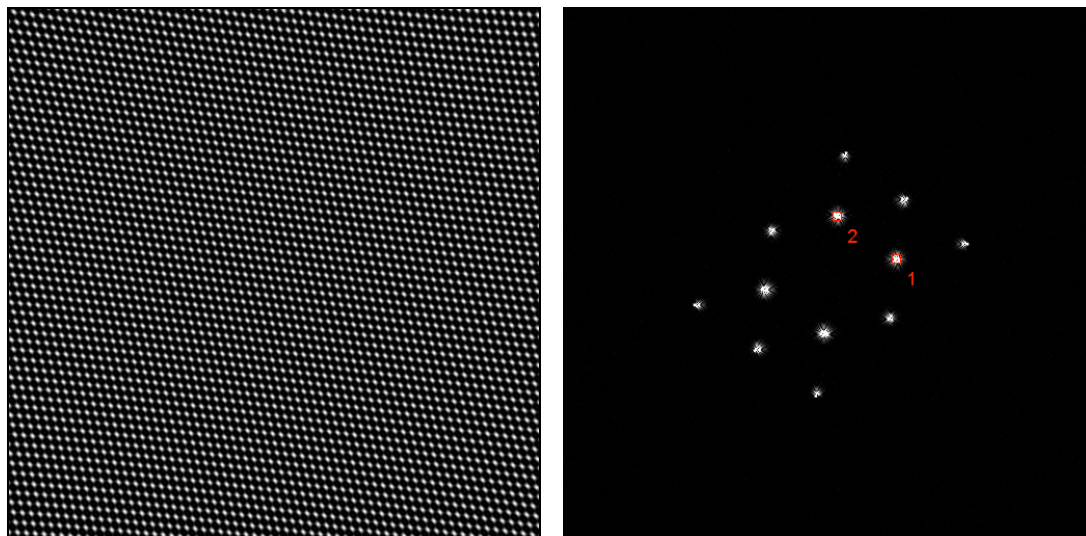
Calculate the two phase images as usual after selecting the spots in the power spectrum:



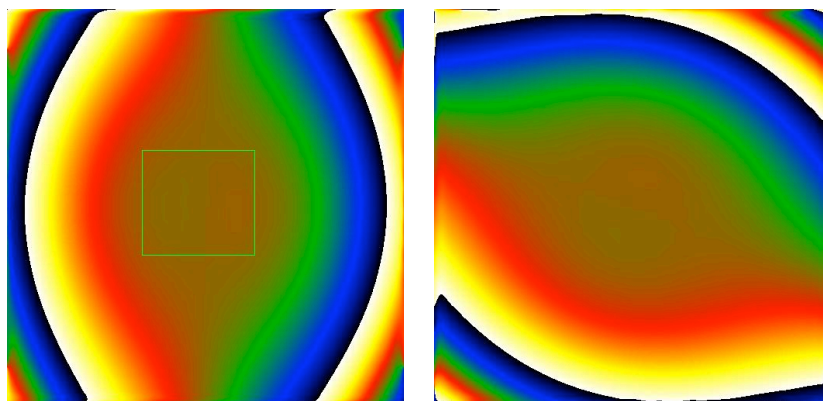
The information contained in the image is dominated by the geometrical distortions.

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*.



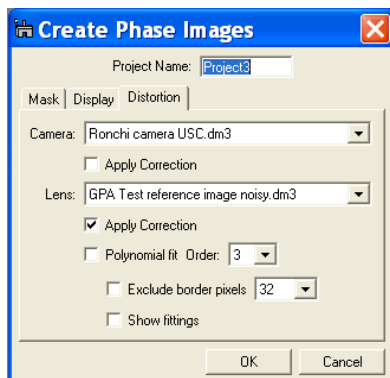
Select two spots and calculate two phase images. In principle, any two non-colinear spots suffice.



Technical note: it is not absolutely necessary to define a reference area but it is good practise.

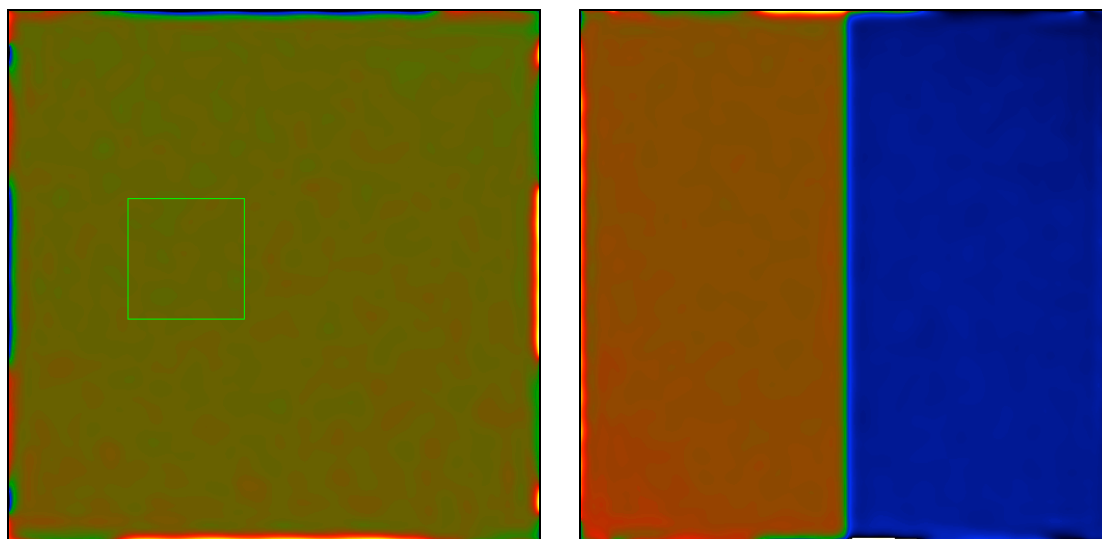
With a phase image selected, use the new menu **Reference Image** and **Save As...** A standard Window's dialog will appear to save a file. By default, a folder is created in *My Images* folder but you can place your reference images anywhere. A good place, if you have administrator rights, is in the 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 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**.

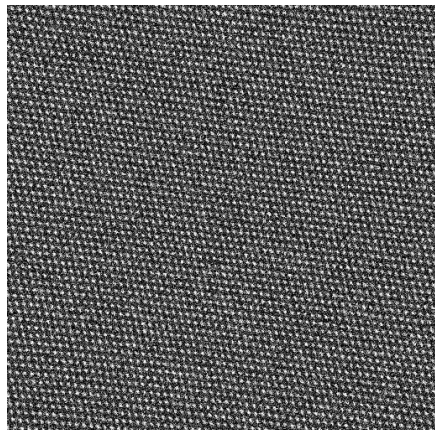
The phase images will automatically be corrected and, after using **Define Reference**, will have a nicely uniform appearance. Only the phase variation due to the crystal structure will be present:



You only need to define the reference image once. From now on, it will be available in the **Phase Calculation...Distortion** tab. If you wish to delete it, just use **Reference Image...Delete**.

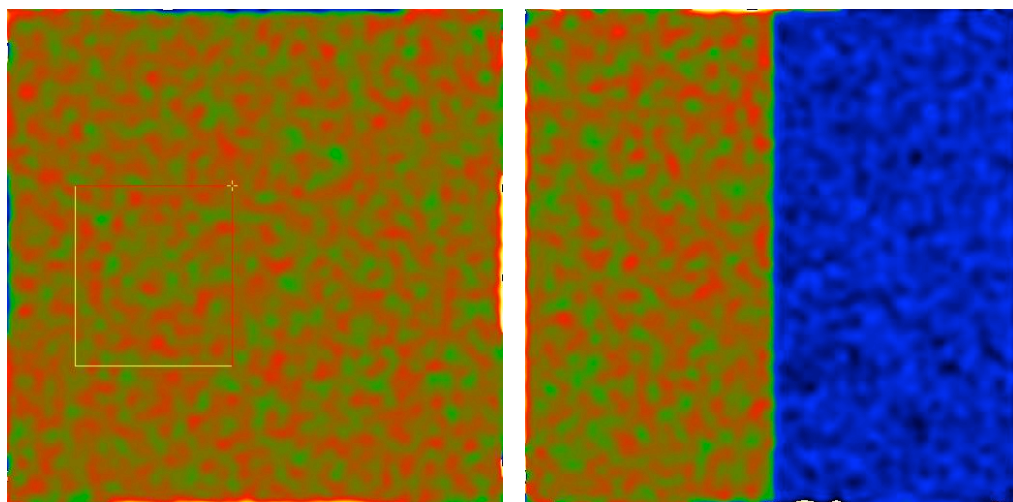
Polynomial fitting

You will not always be so lucky with the reference image. Open the more realistic image *GPA Test reference noisy*:

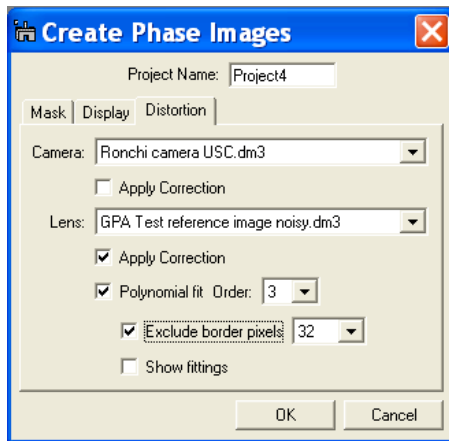


Technical note: this was created simply by adding noise to the previous GPA Test reference image.

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:



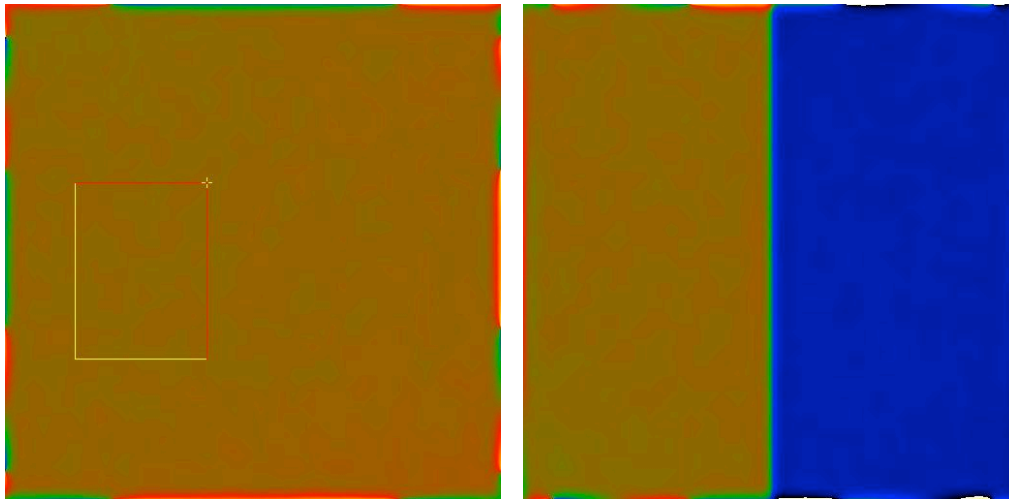
The results are much noisier than the previous example, because the noise in the reference image is effectively added to the image. To alleviate this problem, we have included in GPA Phase 3.0 the possibility of applying a polynomial fit to the reference image phases before subtracting them from the 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!

Appendixes

A: Important phase relations

Phase and displacement:

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

2D displacement and phase:

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

Phase gradient and reciprocal lattice deviation :

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

Strain tensor for small deformations:

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

Mean dilatation :

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

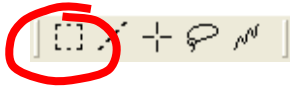
Rotation (in radians and anti-clockwise positive):

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

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:



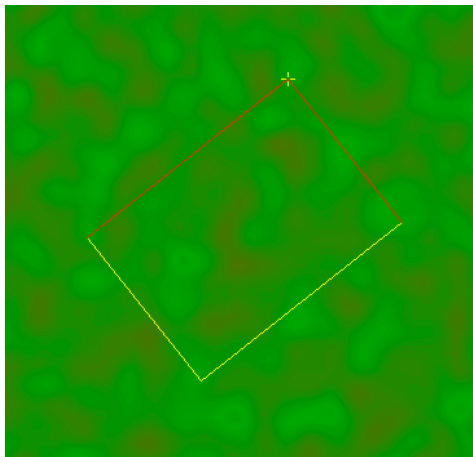
Hint: to select a square area, hold down SHIFT.
To select powers of two, hold down SHIFT-ALT.

DM magnifying glass:



Hint: to demagnify, press ALT.

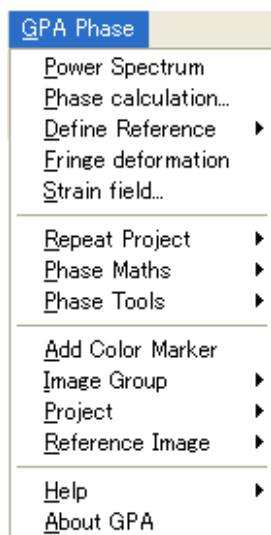
C: Rotatable ROI



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



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.
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).
Strain field...	Calculates the two dimensional deformation tensor. Asks for two phase images and options (see below).
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 to save details of the current project for later use (even in other sessions of DM).

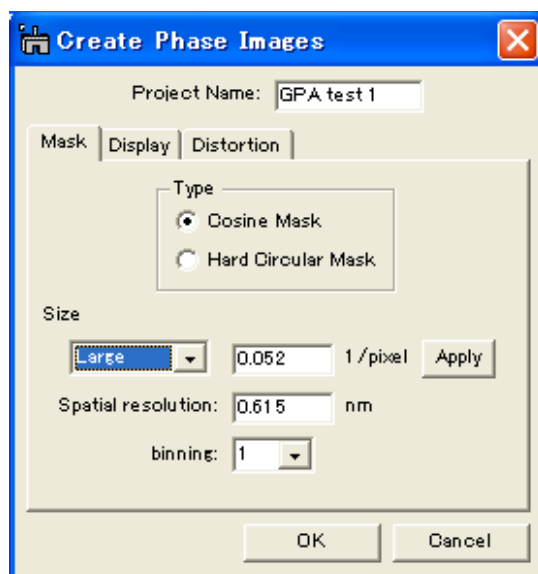
Phase Maths (see sub menus)	Menu of different mathematical operations which can be performed on phase images.
Phase Tools (see sub menus)	Menu of useful operations, not necessarily restricted to phase images.
Add Color Marker	Adds a color bar and the low and high display ranges. You can move the whole 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.
Reference Images (see sub menus)	Menu to define reference images for distortion correction due to CCD cameras or projector lenses.

Phase Calculation Menu

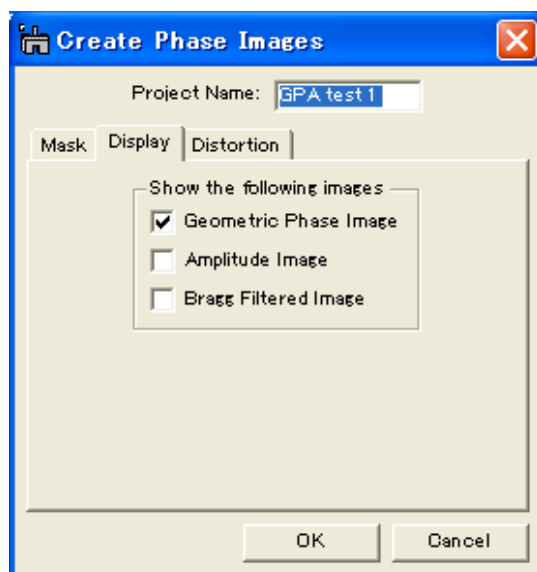
Create Phase Image Dialog

The components of the dialog are described below.

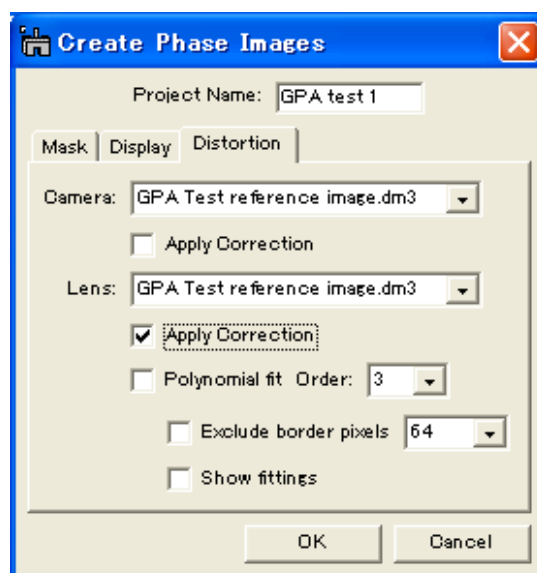
Component	Description
Project Name	Name given to the group of images and results
Mask Tab	For information about the components of the Mask tab, see Mask Tab below.
Display Tab	For information about the components of the Display tab, see Display Tab below.
Distortion Tab	For information about the components 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

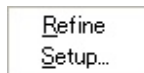
Component	Description
Show the following images	Choice of images to be calculated and displayed.
Geometric Phase Image	Geometric phase image.
Amplitude Image	Amplitude of lattice fringes.
Bragg Filtered Image	Bragg filtered image i.e. image of selected lattice fringes.

Distortion Tab

Option	Description
Camera	Selection of the reference images used for correcting camera distortions (these need preparing with the Reference Image menu).
Lens	Selection of the reference images used for correcting lens distortions (these need preparing with the

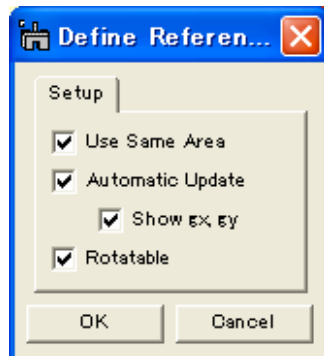
	Reference Image menu).
Apply Correction	Activates the use of the camera and/or lens reference images to correct distortions. If both are activated, the corrections will be applied successively.
Polynomial fit	Activates the use of polynomial fit to the lens distortion (not for camera distortion).
Order	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

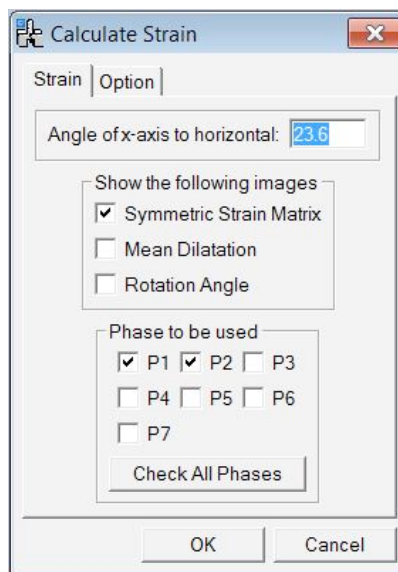


Option	Description
Use Same Area	Reference area is automatically applied to all phase images in the project when using the Refine command or Automatic Update option.
Automatic Update	Moving the reference area automatically updates the phase images and reference values.
Show gx,gy	Displays the values 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

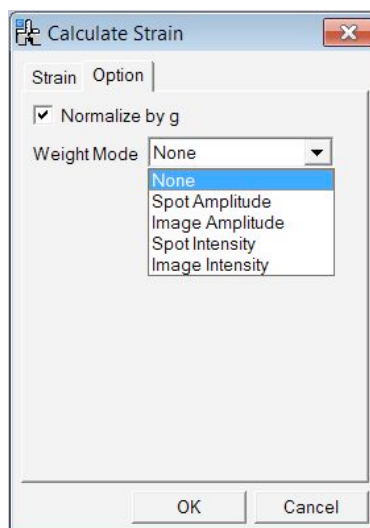
Calculate Strain Dialog (Strain Tab)



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)



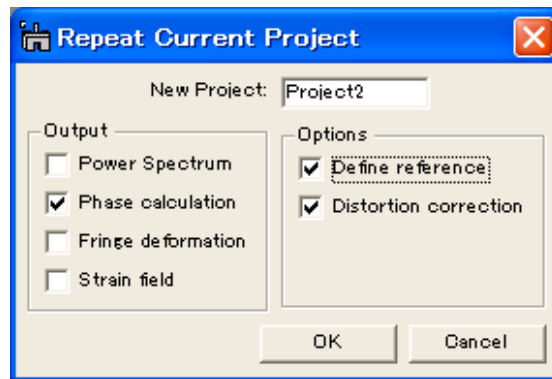
Component	Description
Normalize by g	Applies the weight proportional to 1/g.
Weight Mode	Selection from a weight list: None/Spot Amplitude/Image Amplitude/Spot Intensity/Image Intensity.

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
Invrt 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).

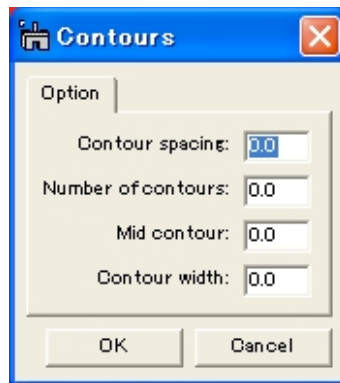
Phase Tools menu



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

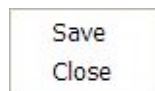
Option	Description
Show gx, gy	Displays in the DM Results window the values of the reference lattice gx and gy in 1/pixels.
Sample by 2	Rebins the front most phase image by two and multiplies the reference by two (thus preserving the reference values gx and gy in pixels ⁻¹ of the newly sampled image).
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)

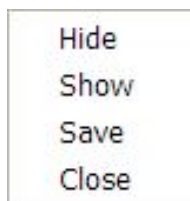


Component	Description
Contour spacing	Step in image values between each contour.
Number of contours	Total number of contours displayed.
Mid contour	Image value corresponding to mid contour.
Contour width	Contour line width in pixels.

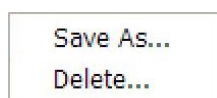
Image Group menu



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.

Reference Image menu

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