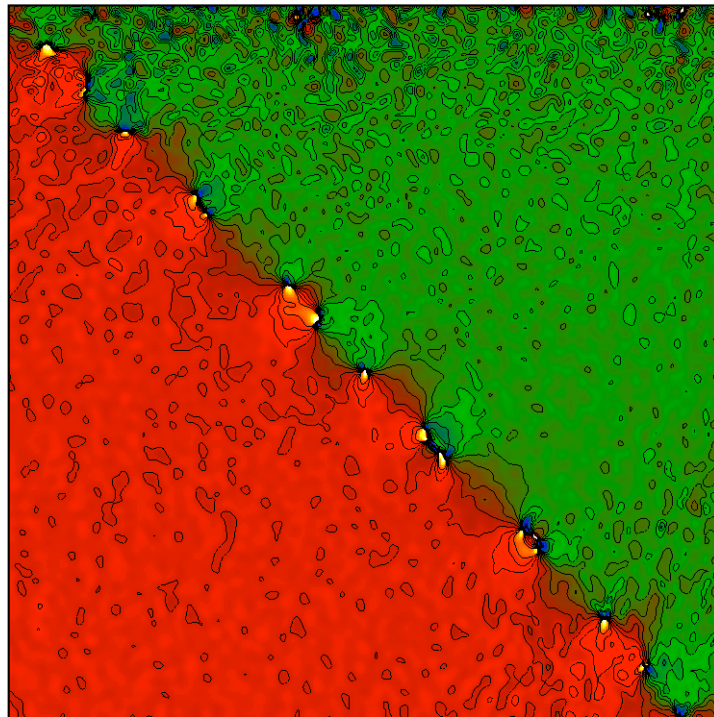


# *GPA for DigitalMicrograph*

## Geometric Phase Analysis



GPA Phase Manual 1.0

HREM Research Inc

## Conventions

The typographic conventions used in this help are described below.

<b>Convention</b>	<b>Description</b>
<b>Bold</b>	Used to denote components of the user interface such as buttons, field names, menus, and menu options.  For example, the <b>New</b> button.
<b>Menu...MenuOption</b>	Select the menu from the menu bar then select the menu option from the menu.  For example, <b>File...Open</b> would mean to select the <b>File</b> menu and then the <b>Open</b> option.
<b>CAPS</b>	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

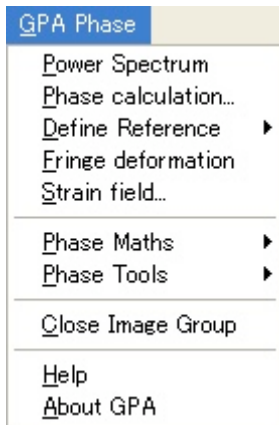
Welcome to GPA Phase the DigitalMicrograph plug-in for strain mapping from high-resolution electron microscope images, or indeed any type of lattice image. There are two main references for the theory:

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

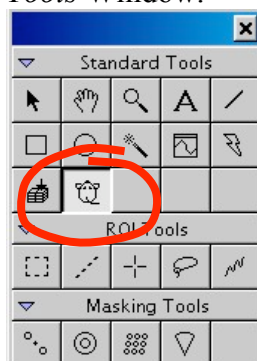
In this manual, we will dive straight into the use of the GPA Phase package with some worked examples. There is also a quick reference guide at the end of this document.

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**:*

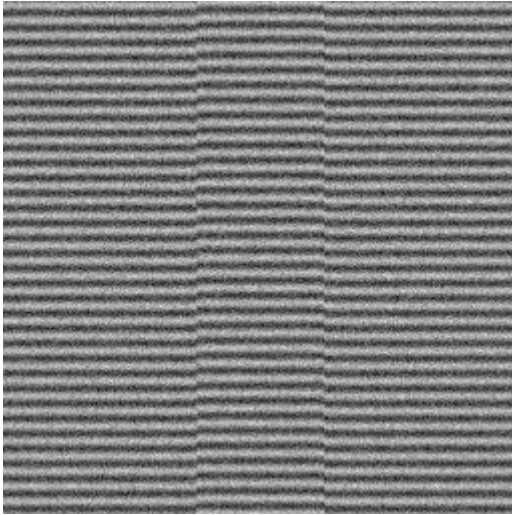


This **mouse tool** is a regular feature of other *HREM Research* plug-ins and is only used in GPA Phase for the selection of spots in the *Power Spectrum*, as we will see.

## GPA Phase Tutorial

### Getting Started

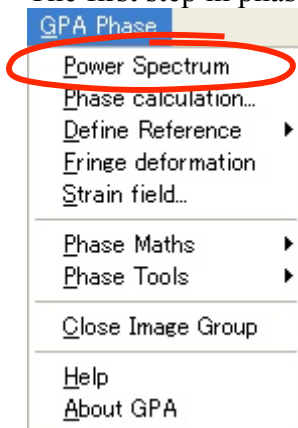
Open the image “GPA Test 0” using the DM command **File...Open** from the GPA Phase Manual folder:



**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.

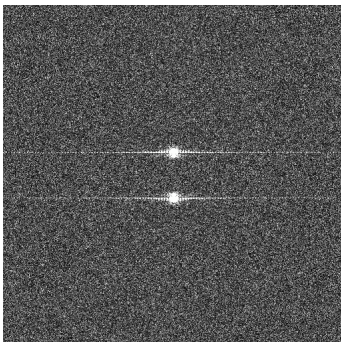
**Hint:** to run a script in DM, press CTRL-ENTER.

The first step in phase analysis is to calculate the *Power Spectrum* of the image:

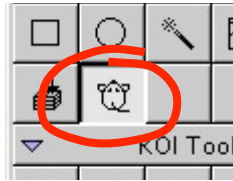


**Technical note:** in GPA, the image does not have to be a power of two in size (e.g. 512 by 512). However, streaks may appear in the power spectrum if greatly different in size from a power of two.

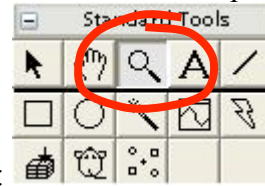
You will see an image similar to this:



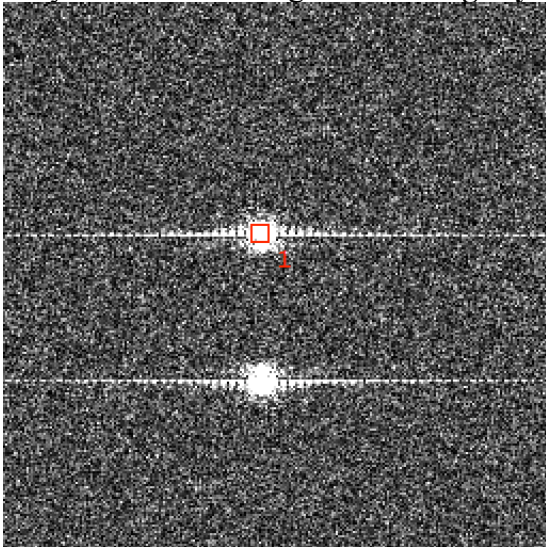
**Technical note:** the power spectrum is the modulus squared of the Fourier transform of the image. People are often surprised by the lack of a central spot in the power spectrum but this is normal for images where the mean intensity is zero, an important difference with diffraction patterns. The horizontal 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:

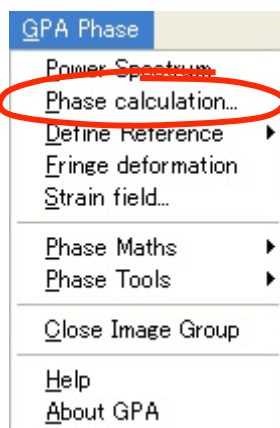


**Technical note:** do not worry about “hitting” the spot exactly. GPA will automatically hunt locally for the maximum intensity in the spot, even though the red square marks the actual pixel you hit.

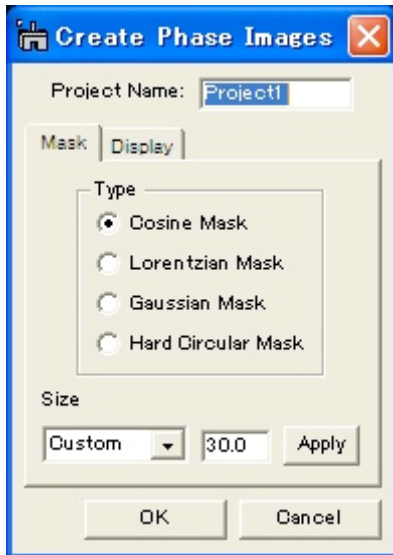
**Hint:** if you wish to delete your mark, click on the mouse mark again with the SHIFT key down, or use the DM **arrow tool** to select and delete.

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*:

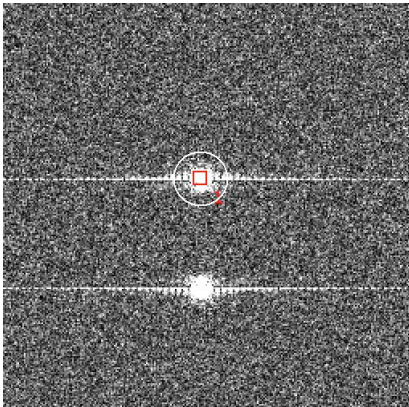


The following dialogue box will appear:



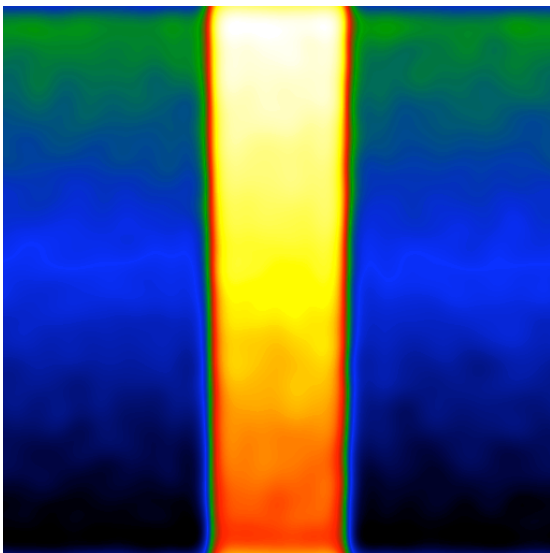
**Technical note:** the choice of the mask type (shape) is not that critical though the hard circular mask is to be avoided (only included for completeness). Hard masks in Fourier space introduce rippling effects in real-space, which is why smooth masks are preferred. Mask size is the most important 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, medium to large. As you do this, the result of your choice will be seen on the *Power Spectrum*:



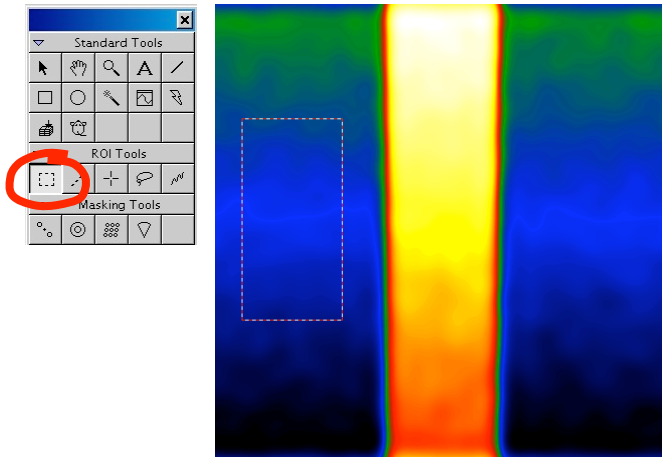
**Technical note:** the radius of the mask shows the area selected in Fourier space around the spot of interest. Decreasing the mask radius will produce smoother results but with less spatial resolution. The maximum recommended size is  $g/2$ .

Now say OK and the phase image will appear:



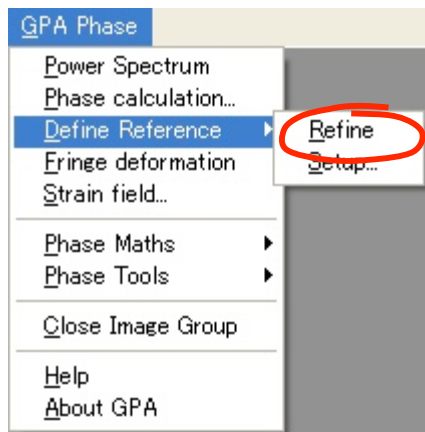
**Technical note:** GPA uses the temperature colour scale for displaying image values. If you prefer grey scales use the DM menu **Object...Image Display...Color**. Similarly, if you wish to change the maximum and minimum display values use DM menu **Object...Image Display...Contrast** or select an area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



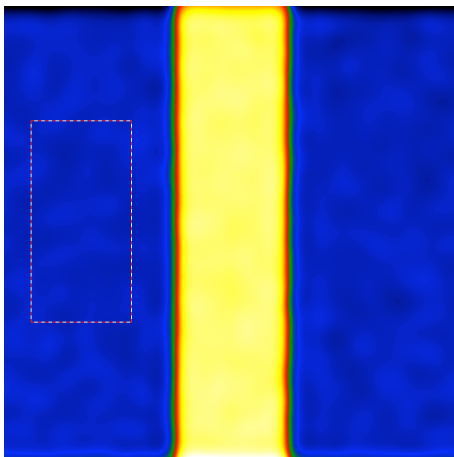
**Technical note:** choose an area of undistorted lattice as your reference area, recognised in the phase image as an area of uniform contrast or uniform gradient. For example, do not choose an area which straddles the interfaces. Having said that, it does not matter to experiment.

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**.

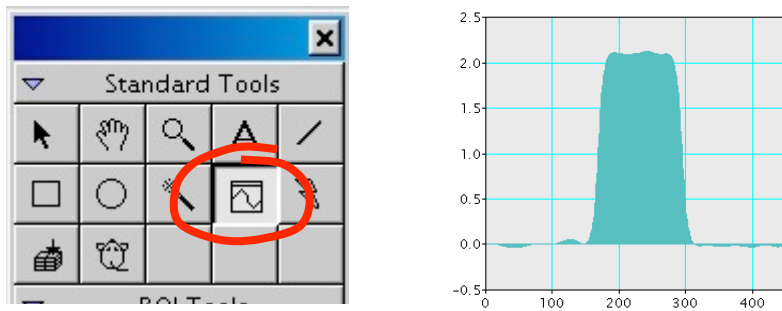
The result will be the following:



**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  $g_x, g_y$** . Values are in  $\text{pixels}^{-1}$

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:

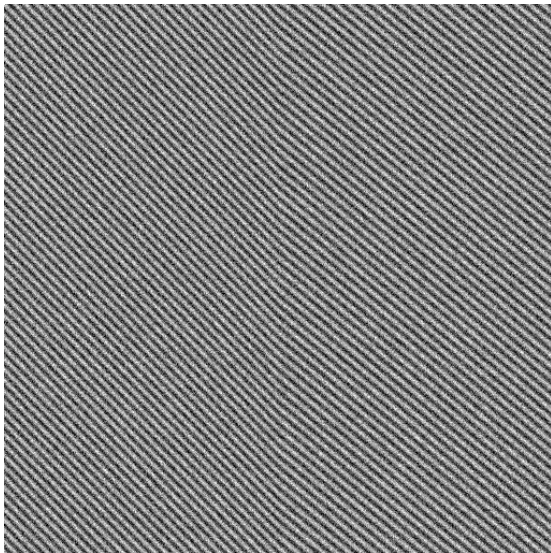


In the reference area the phase is zero and in the central band takes a value of 2.2 radians. This value can be verified in the original script used to create the image “GPA Test image 0”. From the theory, this represents a displacement of  $-2.2/2\pi$  of the lattice spacing. Now choose the reference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

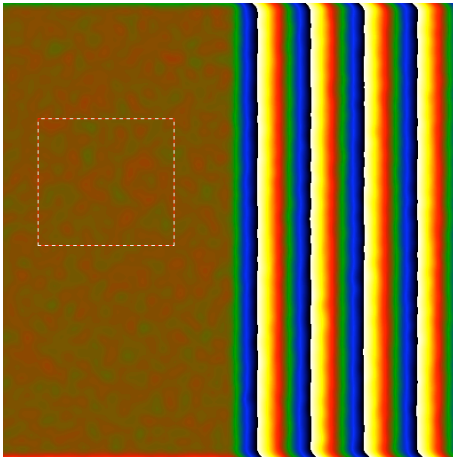
## Fringe deformation mapping

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”:



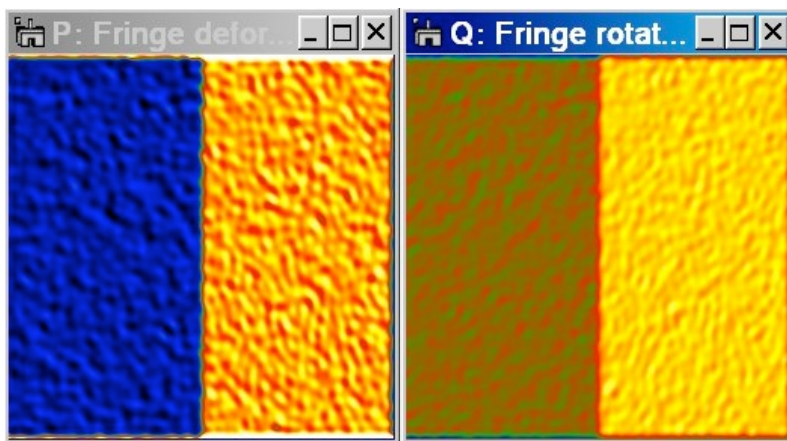
**Hint:** to see the lattice rotation, view the image at a glancing angle to the page. And if you like, try and measure the rotation with standard tools.

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  $\pi$ . Imagine the phase going round a circle moving seamlessly from 0 to  $\pi$  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**:



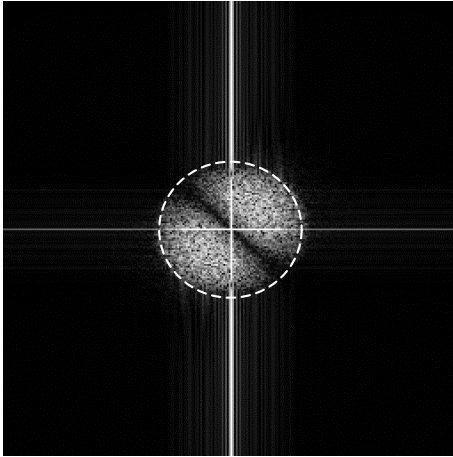
The first image shows the change in lattice spacing relative to the reference lattice in fractional units (i.e. 0.02 means 2% expansion). The paired image shows the rotation of the lattice fringes with respect to the reference in degrees (in-plane rotation of course) and positive anticlockwise. By default 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 can be estimated by looking at the deformation map and taking profiles, for example, or by taking the Fourier transform of the image with **DM Image Processing...FFT.**



**Hint:** when measuring distances and ROI sizes in DM look at the *Control Window*. Values will automatically be in  $\text{pixels}^{-1}$  in image FFTs. For example, use the **circle tool** here.

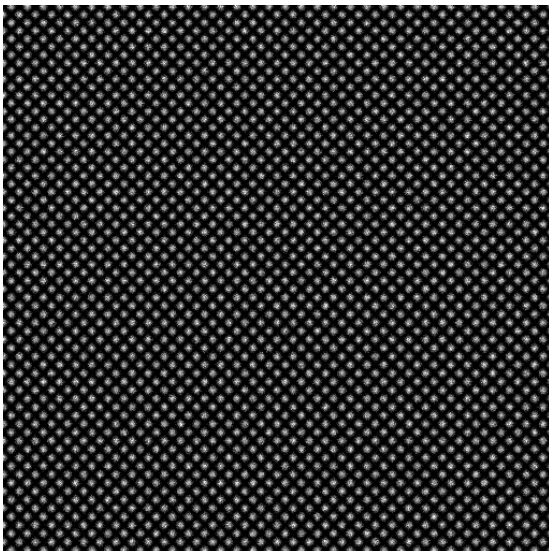
The radius of this circle,  $\kappa$  in  $\text{pixels}^{-1}$ , gives the spatial resolution,  $1/\kappa$  in pixels.

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*.

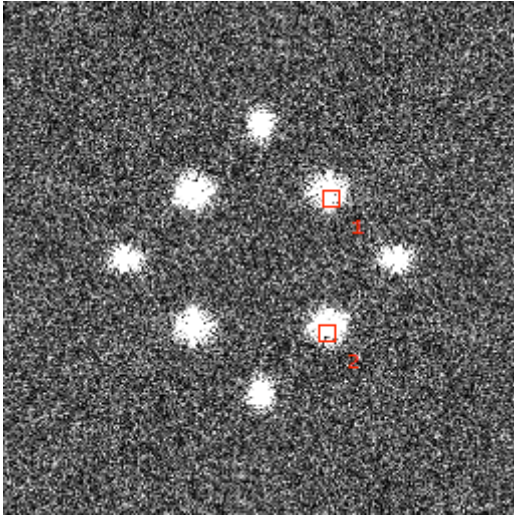
## Determining strain tensors

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”:



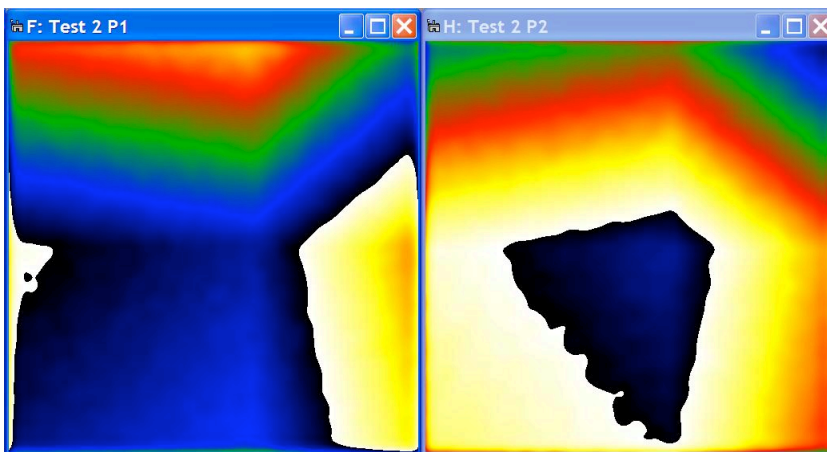
**Technical note:** a deformation is indeed present here, see the script “GPA Test image 2”.

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

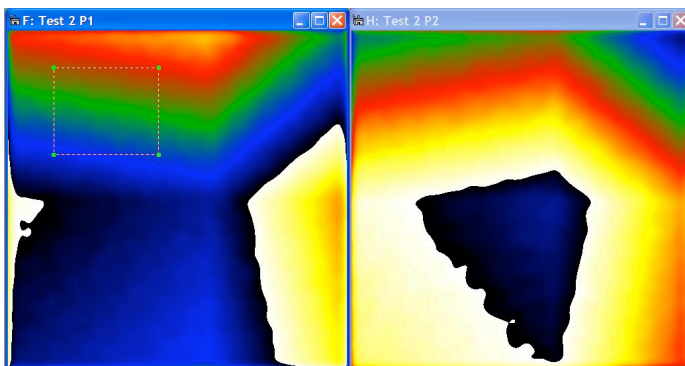


**Technical note:** in principle, it does not matter which two spots you choose, so long as their g-vectors are not parallel. In practice, the highest precision is obtained with low order spots and ones nearest to right-angles with respect to each other. Spots absent in the crystal structure are to be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

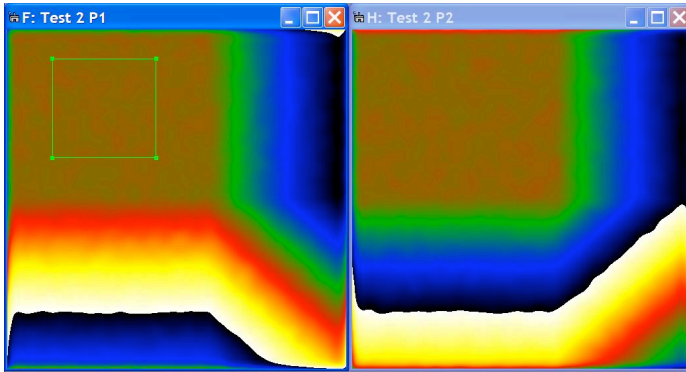


As previously, a reference lattice needs to be defined. This is done by defining an area with the **DM ROI tool** on one of the phase images exactly like the previous examples:



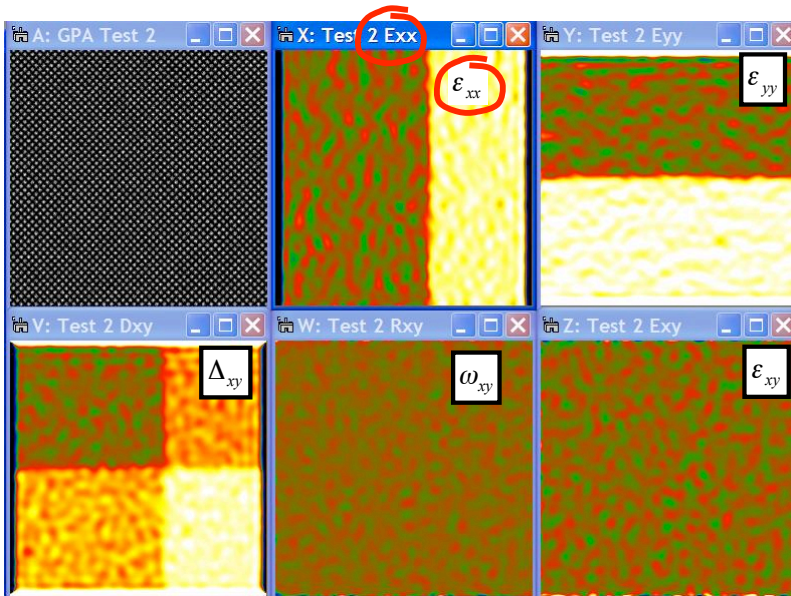
**Hint:** it is not always easy to recognise a good reference region. Just go ahead and try, and if necessary change the selection. Usually the situation becomes clearer after calculating the strain field.

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). Choosing the *x*-axis parallel to the picture horizontal axis (angles anticlockwise positive) and selecting 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 or strain tensor, see the Appendix.

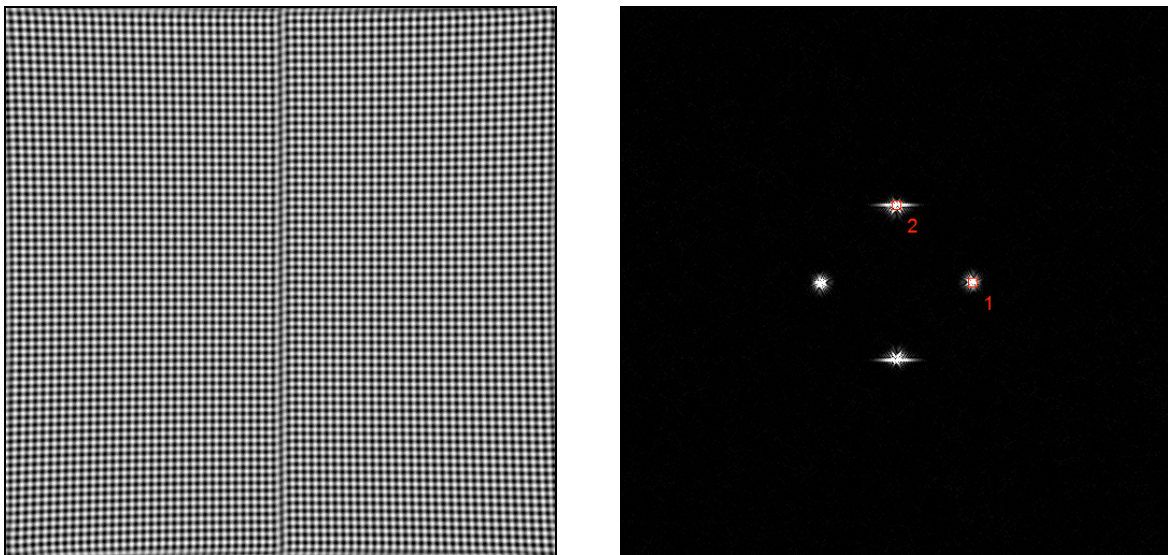
This is the final results of GPA strain analysis: the complete 2-D strain tensor. Now it is your job to enjoy and interpret the results!

## Additional functions

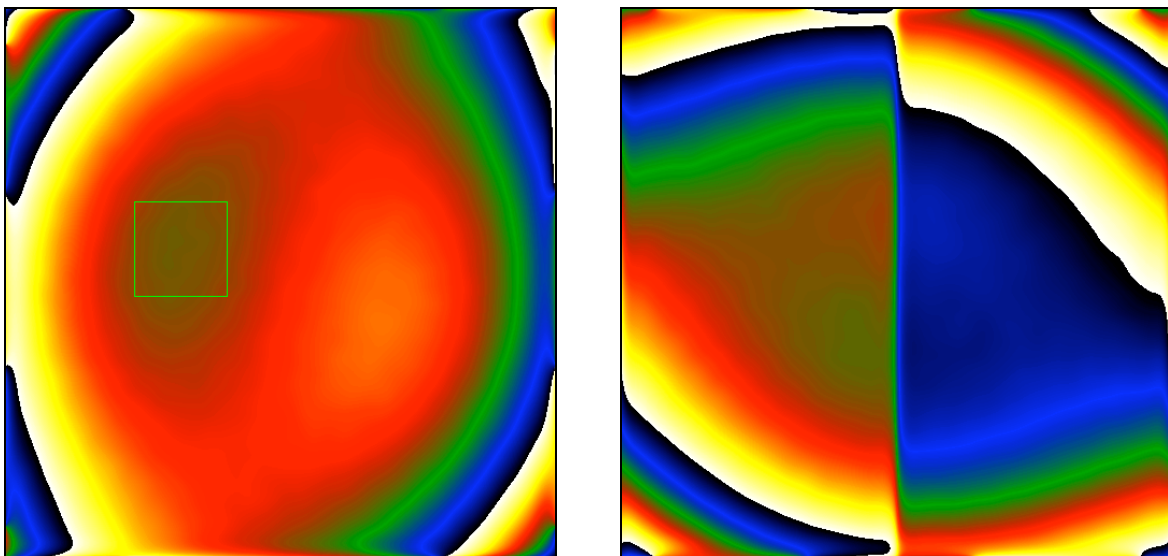
### Geometric distortion correction

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:



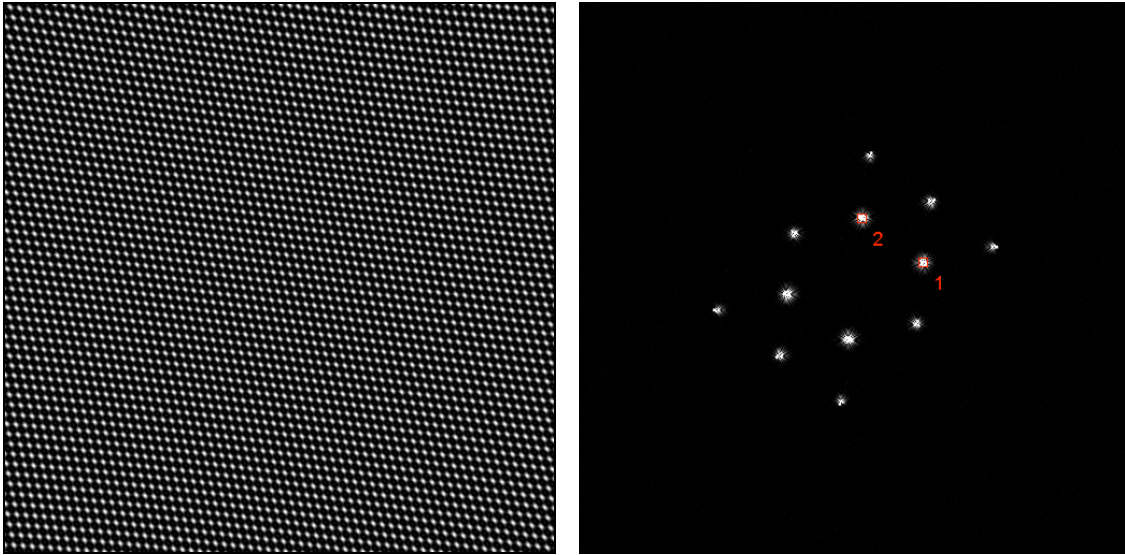
Calculate the two phase images as usual after selecting the spots in the power spectrum:



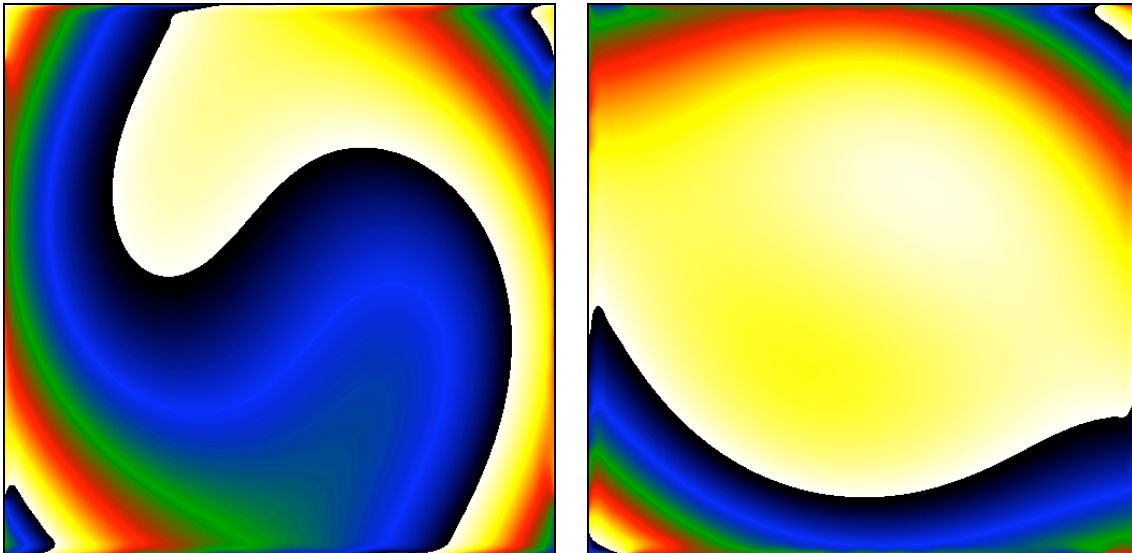
The information contained in the image is dominated by the geometrical distortions.

## Distortion correction

Now open the reference image “GPA reference image” and calculate the *Power Spectrum*.

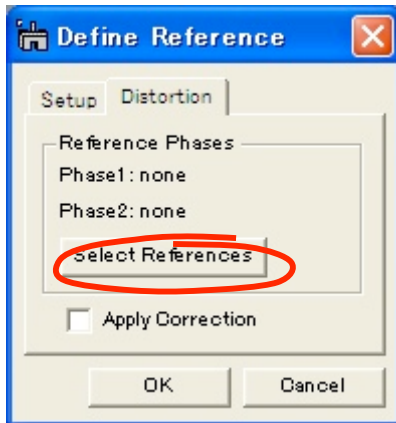


Select two spots and calculate two phase images with a *project name* of Reference for example. In principle, any two non-colinear spots suffice.

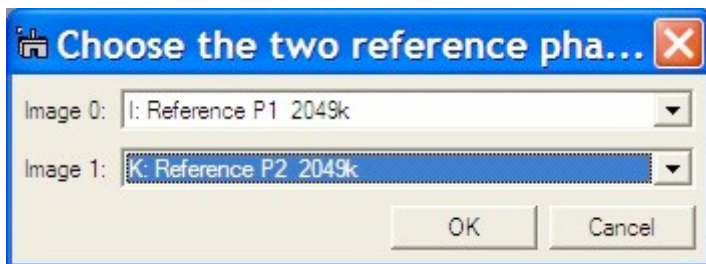


Note: If you save these phase images, you can use them for distortion correction later just by simply opening them.

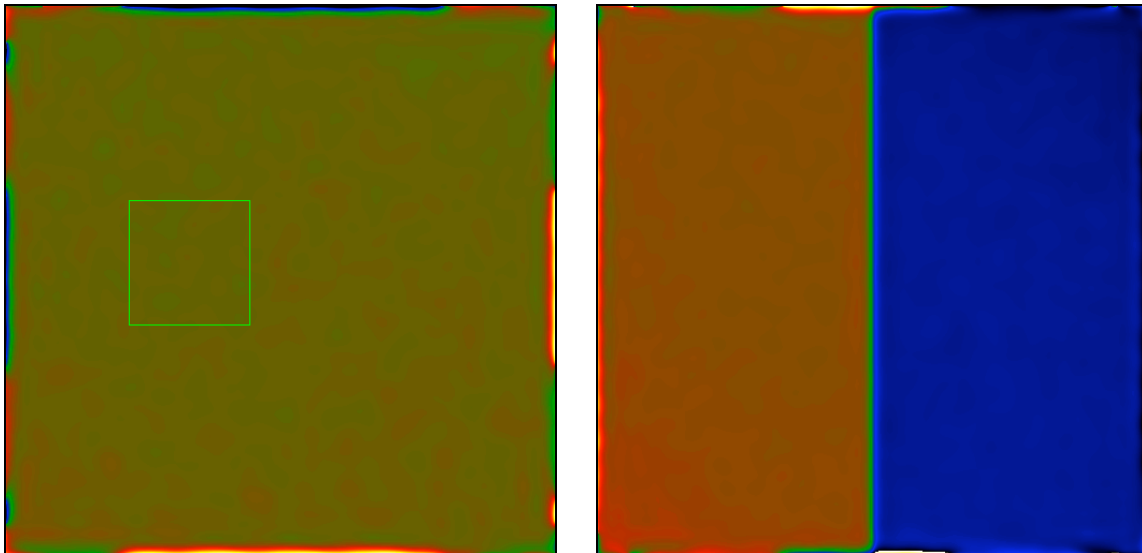
Reselect one of the phase images of “GPA Test distortion”, and place a Rectangular ROI if not present. Then, select **Define Reference...setup** and click on the **Distortion** tab. The following window will appear:



Here, click **Select References** and select the two reference phase images and click **OK**.



Make sure that **Apply Correction** is checked. When you close the **Define Reference** dialog by clicking **OK**, the phase images are automatically corrected:



## 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:

$$\mathbf{u}(\mathbf{r}) = -\frac{1}{2\pi} \left[ P_{g_1}(\mathbf{r})\mathbf{a}_1 + P_{g_2}(\mathbf{r})\mathbf{a}_2 \right] \quad \text{where } \mathbf{g}_i \cdot \mathbf{a}_j = \delta_{ij}$$

Phase gradient and reciprocal lattice deviation :

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

Strain tensor for small deformations:

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

Mean dilatation :

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

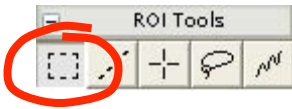
Rotation (in radians and anti-clockwise positive):

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

**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.)

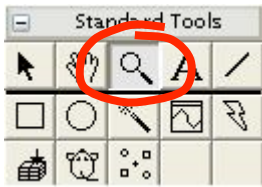
## B: Useful DigitalMicrograph commands

DM ROI tool:



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

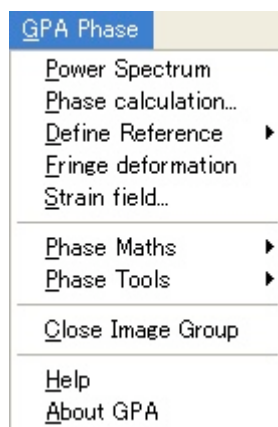
DM magnifying glass:



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

# 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).
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.
Close Image Group	Closes all images of the same nature (and same project) as the front most. Proposes to save before closing.

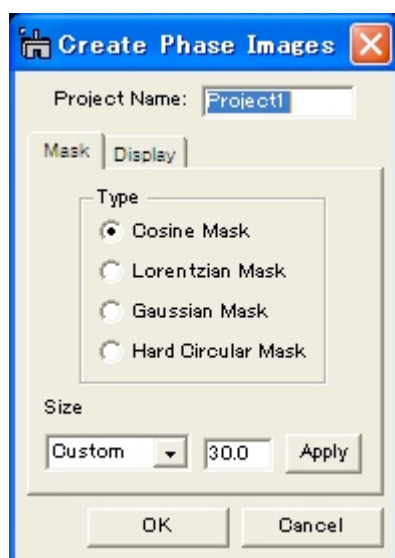
## Phase Calculation Menu

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

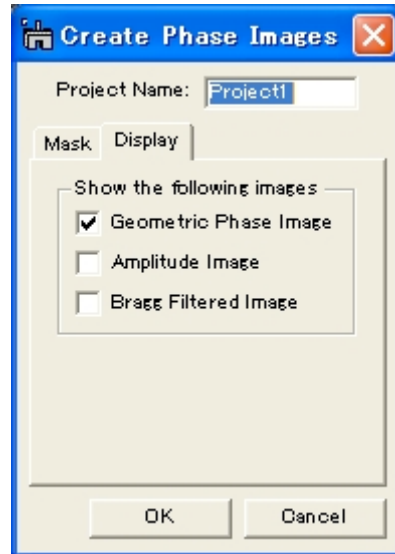
### Mask Tab



Component	Description
Type	Defines the shape of mask used to isolate the selected spots in the Fourier transform.
Cosine Mask	Half-cosine-shaped mask. Size corresponds to radius of hard cut-off and cosine quarter period (i.e. first zero).
Lorentzian Mask	Lorentzian-shaped mask. Size corresponds to radius of hard cut-off and half-width at half size.
Gaussian Mask	Gaussian-shaped mask. Size corresponds to radius of hard cut-off and half-width at half size.
Hard Circular Mask	Top-hat function. Size corresponds to radius of hard cut-off.
Size	Defines mask width and 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.

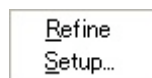
Text Field	In units of pixels in the FFT.
Apply Button	Displays mask size as circles on Power Spectrum around selected spots.

### Display Tab

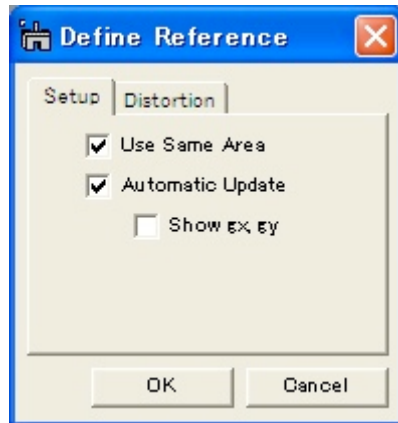


Component	Description
Display	Choice of images to be calculated and displayed.
Geometric Phase Image	Geometric phase image.
Amplitude Image	Amplitude of lattice fringes.
Bragg Filtered Image	Bragg filtered image i.e. image of selected lattice fringes.

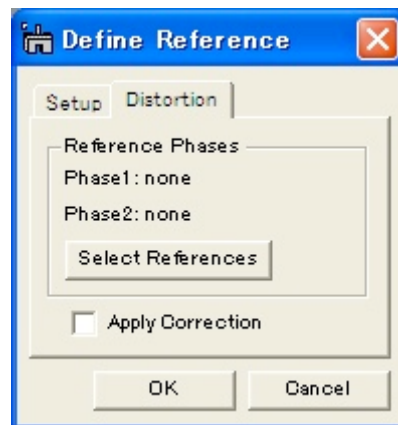
### Define Reference Menu



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 adjusts phase images accordingly (see options).
Setup...	Options menu.

**Setup Tab**

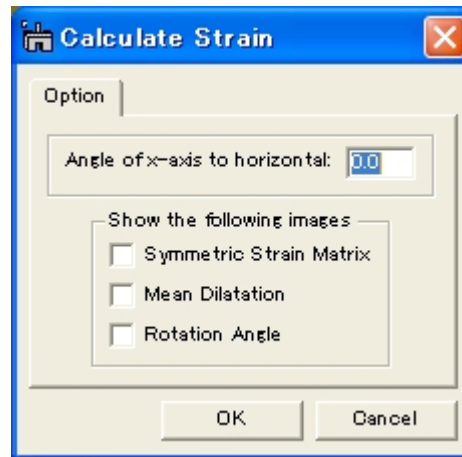
Option	Description
Use Same Area	Reference area is automatically applied to all phase images in the project when using the Refine command or Automatic Update option.
Automatic Update	Moving the reference area automatically updates the phase images and reference values.
Show gx,gy	Displays the values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

**Distortion Tab**

Option	Description
Reference Phases	Phase images used for correcting distortions.
Select References	Button allowing the selection of the two reference phases from a list of open images.
Apply Correction	Activates the use of the reference phases to correct distortions.

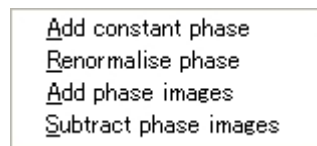
## Strain Field Menu

### Calculate Strain Dialog (Option Tab)



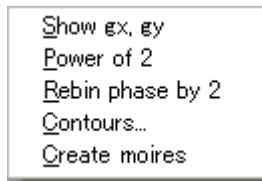
Component	Description
Angle of x-axis to horizontal	Defines the orientation of the x-axis used for the strain calculation. Angle defined in degrees from the horizontal plane of the image to the x-axis (anticlockwise positive).
Show the following Images	Choice of results to be displayed.
Symmetric Strain Matrix	Images of $\epsilon_{xx}$ , $\epsilon_{yy}$ and $\epsilon_{xy}$ to be displayed.
Mean Dilatation	Image of $\delta_{xy}$ to be displayed (average of $\epsilon_{xx}$ and $\epsilon_{yy}$ ).
Rotation Angle	Image of $\omega_{xy}$ to be displayed. Values in degrees and anticlockwise positive.

## Phase Maths Menu



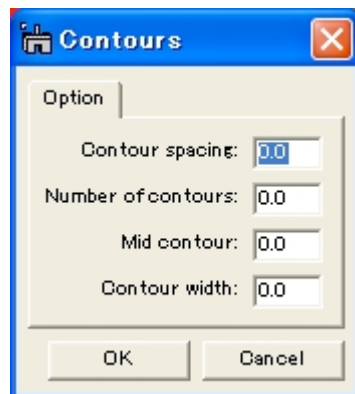
Option	Description
Add constant phase	Adds a uniform phase value to the front most image and renormalizes the phase.
Renormalize phase	Renormalizes the phase between $-\pi$ and $+\pi$ .
Add phase images	Adds two phase images together (requested in a dialog box) and displays result in a third window (after phase renormalization). New phase image also has a reference equal to the sum of the references of the two phase images.
Subtract phase images	Subtracts two phase images (requested in a dialog box) and displays result in a third window (after phase renormalization). New phase image also has a reference equal to the difference between the references of the two phase images.

## Phase Tools Menu



Option	Description
Show gx, gy	Displays in the DM Results window the values of the reference lattice gx and gy in 1/pixels.
Power of 2	Pastes the front most image into an image of dimensions equal to a power of two. Blank space is filled with mean intensity.
Rebin phase 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 <sup>-1</sup> of the newly sampled image).
Contours...	Superimposes contours on the front most image (see options).
Create moires	Creates a moiré image from the front most phase image. Asks for the magnification factor n equivalent to moiré fringes every n lattice fringes.

## 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.