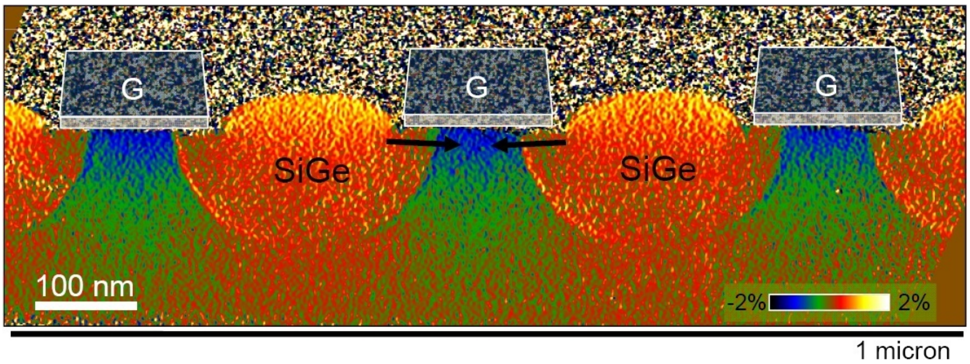
2014/04/15

HoloDark for DigitalMicrograph

Dark-field Electron Holography Analysis for Strain Mapping

Patent N° US 8,502,143 B2



HoloDark Manual 1.3

HREM Research Inc

Conventions

The typographic conventions used in this help are described below.

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

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HoloDark US Patent : Patent N° US 8,502,143 B2

Copyright Statements

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

Software requirements

The following is a list of the software requirements necessary to run the HoloDark 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 HoloDark, or you can find it on our web site.

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

Introduction to HoloDark

Welcome to the HoloDark plug-in for DigitalMicrograph. The software provides both the analysis for creating strain maps from dark-field electron holograms (DFEH) and the rights to use this patented technique. Here are the relevant references:

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

[2] M.J. Hÿtch, F. Houdellier, F. Hüe, and E. Snoeck, **Ultramicroscopy** 111 (2011) 1328–1337. *Dark-field electron holography for the measurement of geometric phase. 10.1016/j.ultramic.2011.04.008*.

[3] M.J. Hÿtch, F. Houdellier, F. Hüe, and E. Snoeck, **United States Patent** N° US 8,502,143 B2**,** 6th August 2013. *Method, device and system for measuring nanoscale deformations*. CNRS.

The analysis is based on measuring the geometric phase of electrons passing through deformed regions of crystal, directly from the dark-field electron holograms. The strain is then determined from the geometric phase as described in the following reference:

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

In addition to the above, applications of HoloDark can be found in the following:

[5] M. J. Hÿtch, F. Houdellier, F. Hüe and E. Snoeck, **Journal of Physics**: Conference Series 241 (2009) 012027. *Dark-field electron holography for strain mapping in nanostructures: correcting artefacts and aberrations*. doi:10.1088/1742-6596/241/1/012027.

[6] F. Hüe, M.J. Hÿtch, F. Houdellier, H. Bender, and A. Claverie, **Appl. Phys. Lett**. 95, 073103 (2009). *Strain mapping of tensiley strained silicon transistors with embedded $Si_{1-y}C_y$ source and drain by dark-field holography. doi:10.1063/1.3192356*.

[7] N. Serra, F. Conzatti, D. Esseni, et al., **Proc. IEDM 2009** (IEEE International). *Experimental and physics based modeling assessment of strain induced mobility enhancement in FinFETs. 10.1109/IEDM.2009.5424419*.

[8] S. Reboh, P. Benzo, P. Morin, R. Cours, M. J. Hÿtch, and A. Claverie, **Appl. Phys. Lett.** 102, 051911 (2013). *A method to determine the Young's modulus of thin-film elements assisted by dark-field electron holography. 10.1063/1.4790617*.

[9] N. Cherkashin, S. Reboh, M.J. Hÿtch, A. Claverie, V.V. Preobrazhenskii, M.A. Putyato, B.R. Semyagin, and V.V. Chaldyshev, **Appl. Phys. Lett.** 102, 173115 (2013). *Determination of stress, strain, and elemental distribution within In(Ga)As quantum dots embedded in GaAs using advanced transmission electron microscopy. 10.1063/1.4804380*.

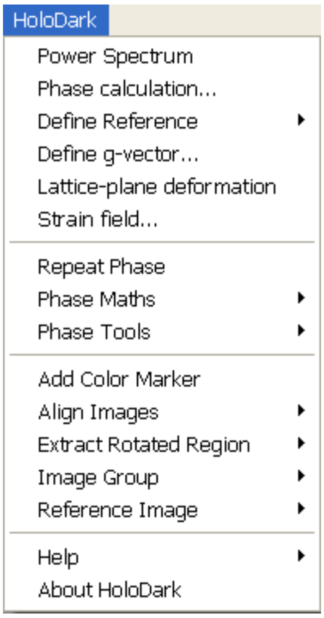
And a theoretical paper about the propagation of geometric phase through 3D strain fields:

[10] A. Lubk, E. Javon, N. Cherkashin, S. Reboh, C. Gatel, and M.J. Hÿtch, **Ultramicroscopy** 136, 42-49 (2014). *Dynamic scattering theory for dark-field electron holography of 3D strain fields. 10.1016/j.ultramic.2013.07.007*.

In this manual, we will dive straight into the use of the HoloDark 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. *HoloDark 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 HoloDark variables will not be transferred.
2. *All the commands related to HoloDark* are located in the menu **HoloDark**:



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 HoloDark for the selection of spots in the *Power Spectrum*, as we will see.

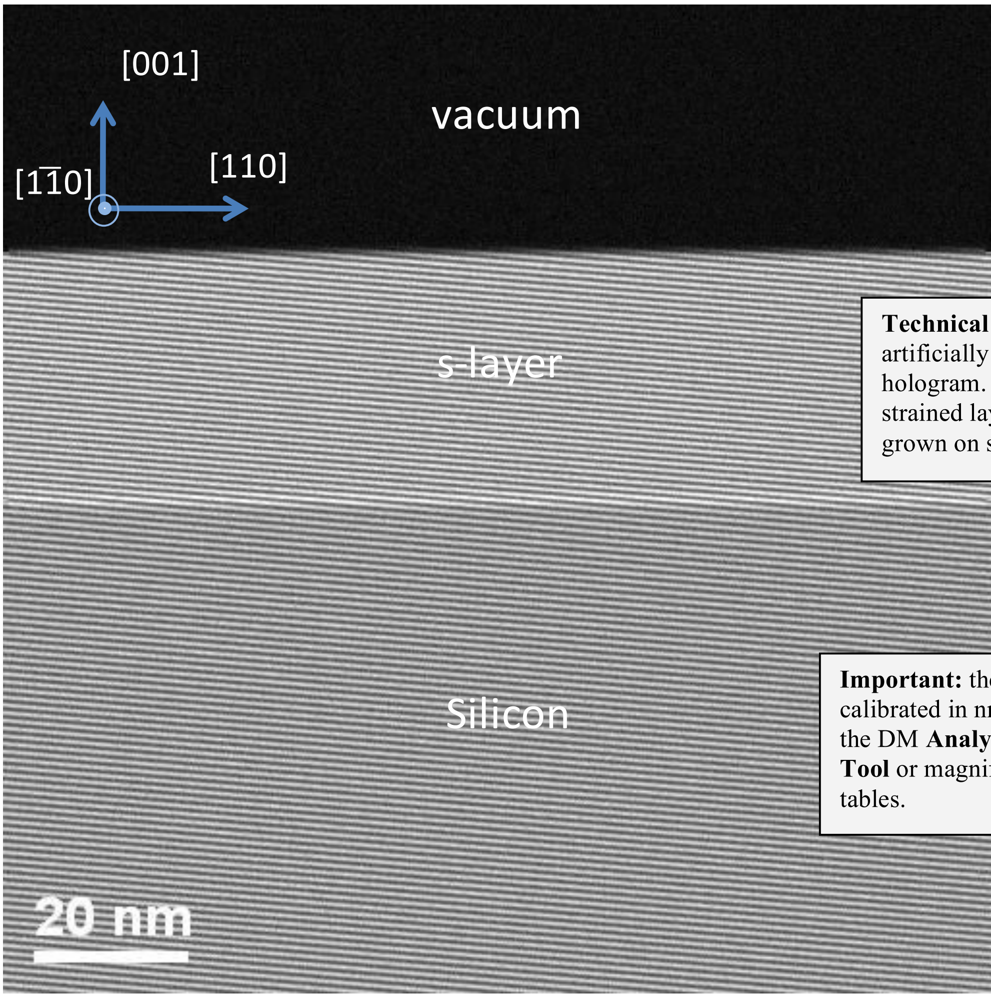
New features of version 1.3

HoloDark 1.3 has the possibility of defining tetragonal and orthorhombic crystalline lattices in addition to cubic. The crystal settings can also be saved for later use.

HoloDark Tutorial

Getting Started

Open the hologram image “Thin layer h004” using the DM command **File…Open** from the HoloDark Manual folder:



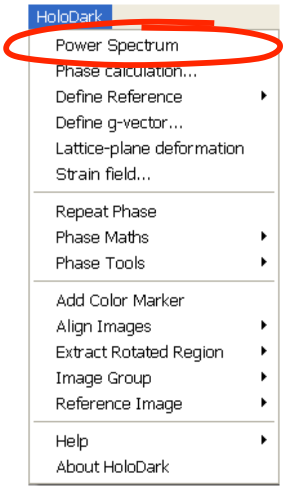
Technical note: this is an artificially constructed hologram. It represents a strained layer of material grown on silicon.

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

This is a hologram made from the interference of the (004) diffracted beam from the substrate (in this case monocrystalline silicon) with the (004) beam from the strained layer. Notice that there are no holographic fringes in the vacuum – the true sign of dark-field holography (DFEH). The crystallographic orientation of the sample will be important for the analysis, including the signs of the indices (**g** or –**g** for example). In these examples, we assume that the microscopist carrying out the experiments (which may or may not be you!) has supplied the necessary information, notably:

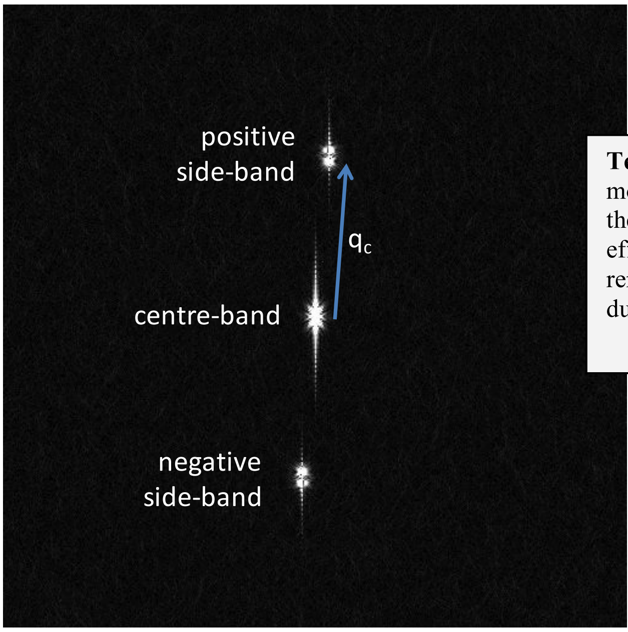
- the exact indices of the diffracted beam used,
- the zone axis,
- the in-plane orientation of the sample,
- and the magnification of the image.

Firstly, you need to verify that the image has been correctly calibrated, in our case indicated by the presence of a scale marker. Now you are ready to start and to calculate the *Power Spectrum* of the image:



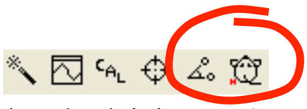
Technical note: in HoloDark, the image does not have to be a power of two in size (e.g. 512 by 512). However, streaks may appear in the power spectrum if greatly different in size from a power of two.

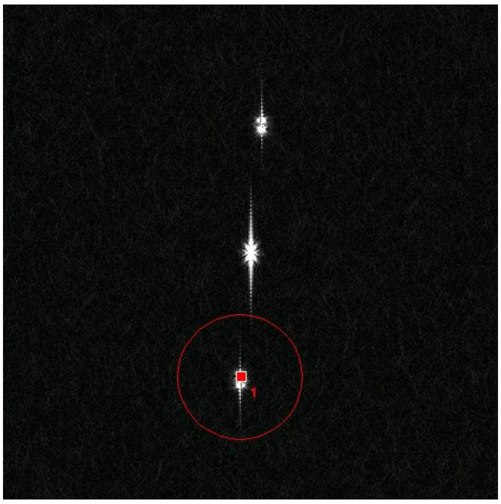
You will see an image similar to this:



Technical note: the power spectrum is the modulus squared of the Fourier transform of the hologram. To avoid streaking from edge effects, the hologram was prefiltered. The remaining vertical streaking of the spots is due to the interfaces and is not an artefact.

The Fourier transform consists of what is called a "centre band", which represents variations in the background intensity in the hologram, and two "side bands" which contain the information on the holographic fringes, and hence the strain. The reciprocal vector which corresponds to the side-band frequency is called the "carrier frequency", $\mathbf{q}_c$, and points from the reference (the substrate) to the measurement area (the stained layer). The holographic fringes spacing, d_c, is $1/q_c$.

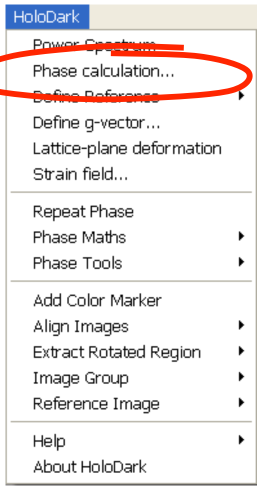
Now choose the **mouse tool**:  and click on the side-band towards the bottom, the negative side-band. Indeed, it is **very important** in HoloDark to remember to choose **the side-band pointing towards the substrate** i.e. in the direction of the reference area with respect to the measurement area. Choosing the other will result in an error of sign in the strain results – compression becoming tension and vice-versa.



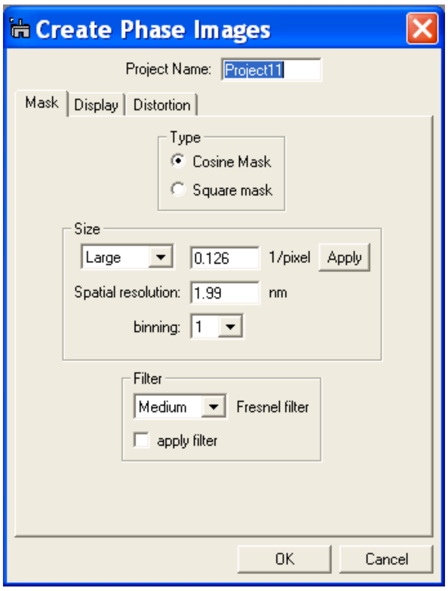
Technical note: do not worry about “hitting” the spot exactly. HoloDark will automatically hunt locally for the maximum intensity in the spot, even though the red square marks the actual pixel you hit.

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.

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

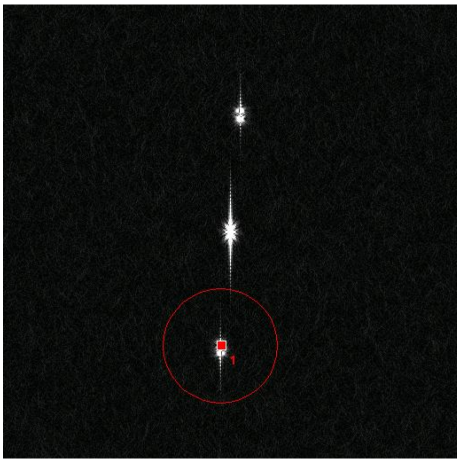


The following dialogue box will appear:



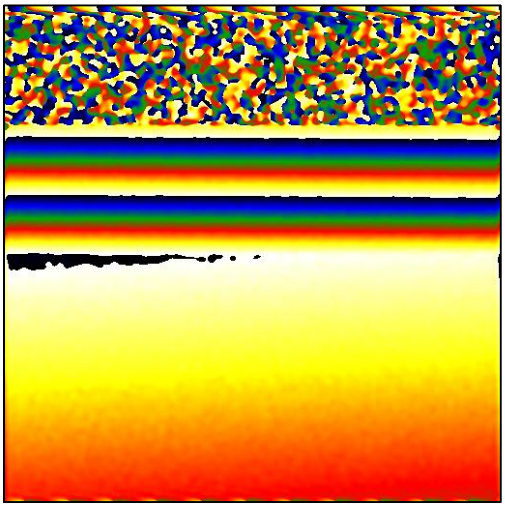
Technical note: in general we recommend the *Cosine Mask*. The *Square Mask* has been included as an option. The most important parameter is the mask size which determines the spatial resolution of the results.

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

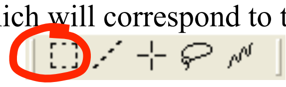


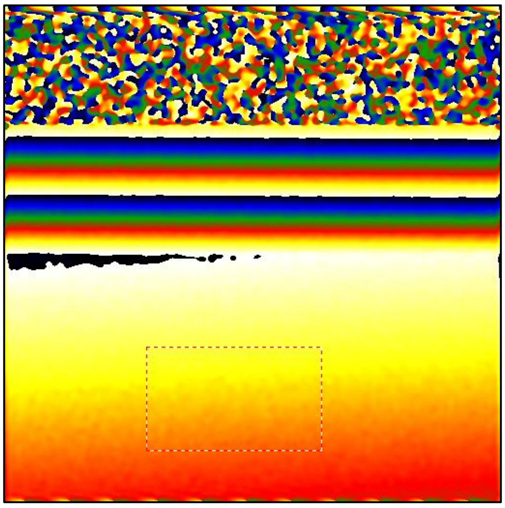
> **Technical note:** the radius of the mask shows the area selected in Fourier space around the spot of interest. Decreasing the mask radius will produce smoother results but with less spatial resolution. The maximum recommended size is $q_c/2$ corresponding to the large mask size – the default value – and corresponds to a spatial resolution of $2d_c$.

Now say OK and the phase image will appear:



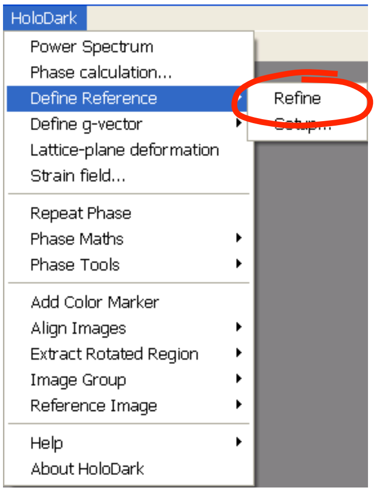
> **Technical note:** HoloDark uses the temperature colour scale for displaying image values. If you prefer grey scales use the DM menu **Object…Image Display…Color**. Similarly, if you wish to change the maximum and minimum display values use DM menu **Object…Image Display…Contrast** or select an area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

The next step is to define area which will correspond to the reference lattice. Use the DM **ROI tool** (region of interest tool)  to select and area:

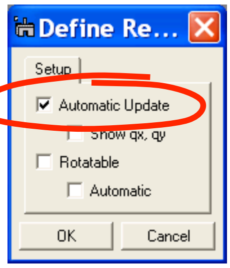


> **Technical note:** choose an area of undistorted lattice as your reference area, recognised in the phase image as an area of uniform contrast or uniform gradient. For example, do not choose an area which straddles the interfaces. Having said that, please experiment.

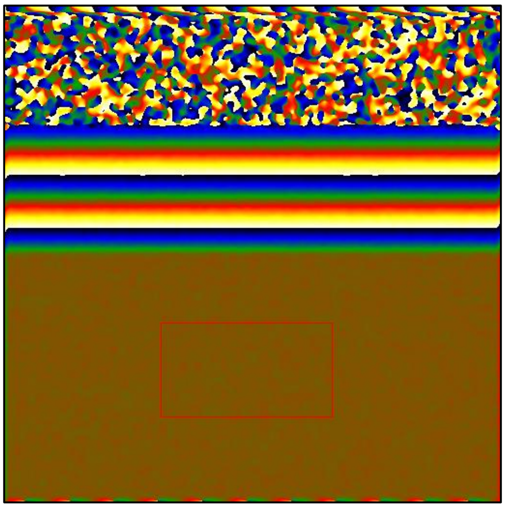
and choose the next HoloDark command **Define Reference**.



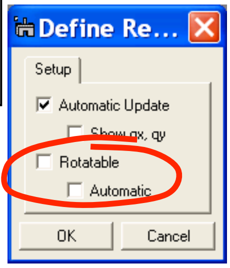
> **Hint:** if you do not like the reference area, just grab and slide the ROI across the image. HoloDark will automatically update the reference area. This function can be deactivated in **Define Reference…Setup**.



The result will be the following:



> **Hint:** if you find the box is rotated, deactivate this function for the moment in the **Define Reference…Setup**.



The phase image now has a well defined reference lattice. Do not worry about the "phase jumps" i.e. where the phase suddenly goes from black to white. This is quite normal and results from the normalisation of the phase between $-\pi$ and 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 holographic fringes.

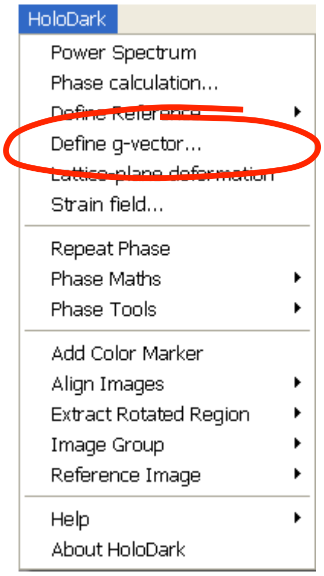
The uniform area of phase shows the substrate (here in brown). The strained layer shows up as a region of varying phase (in this case with a linear gradient). The gradient of the phase will determine the difference in lattice parameter and crystal orientation of the (004) lattice planes.

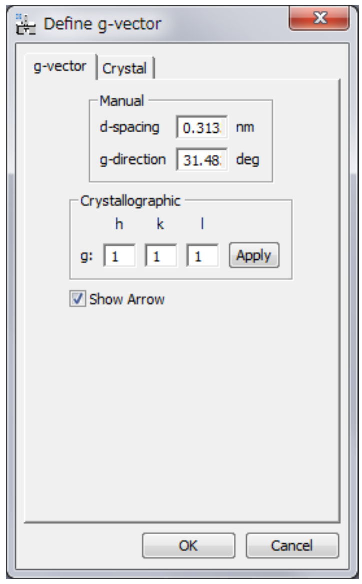
Here is the recommendation for the choice of reference area:

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

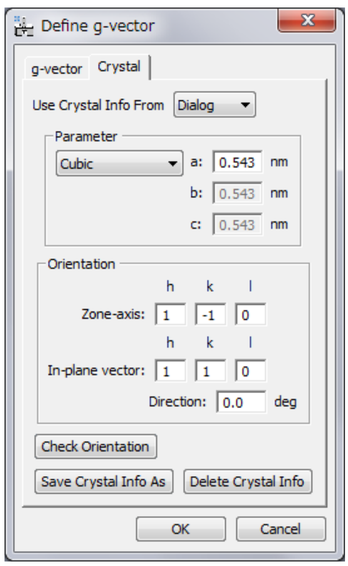
Diffraction vectors and crystallography

DFEH analysis requires knowledge of the specimen crystallography and orientation, and more specifically the exact value and direction of the g-vector used to create the hologram. To enter these, use the HoloDark command **Define g-vector…**:





Firstly, you need to define the reference crystal you are working with using the **Crystal** tab:



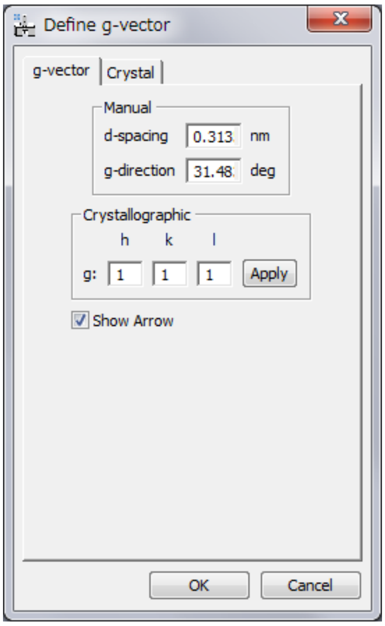
Technical note: for the moment HoloDark can only deal with cubic, tetragonal and orthorhombic crystals.

The example is Silicon, which is cubic with a lattice parameter of 0.543 nm, as shown. The zone-axis is [1-10] as defined pointing up and out of the plane of the hologram (see annotations on the hologram at the start of the tutorial). You now need to give the program the orientation of any one in-plane g-vector, not necessarily the diffraction vector used.

If "Use Crystal Info from" is "Dialog," the crystal setting currently shown in the dialog will be used. You can save/delete the crystal setting and use it later.

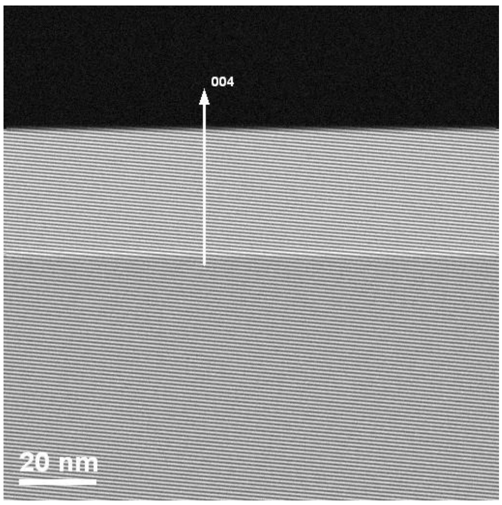
For strained-silicon structures, the [110] direction is often easily identified in the image, or indeed the growth direction [001]. Here the [110] direction has been entered, which is parallel to the interface between the substrate and the layer. The direction means the angle between the in-plane vector and the image horizontal (anticlockwise positive). You can use DM **line ROI** tools to measure this from the image. In this case, the answer is easy (zero). Naturally, you are at liberty to define your own coordinate system, for example with the positive [110] direction as being at 180° i.e. the opposite direction. However, for the rest we will assume the above orientation.

After defining the reference crystal, click on the **g-vector** tab:



> **Technical note:** as mentioned above, you can define manually the g-vector by directly tapping values in the **Manual** box. However, mistakes are more readily avoided by using the **Crystallographic** settings when possible.

In this case the diffracted beam was the (004) so change the g (hkl) indices accordingly, and press on the **Apply** button. With the **Show Arrow** box ticked, you should see an arrow appearing on the hologram image:

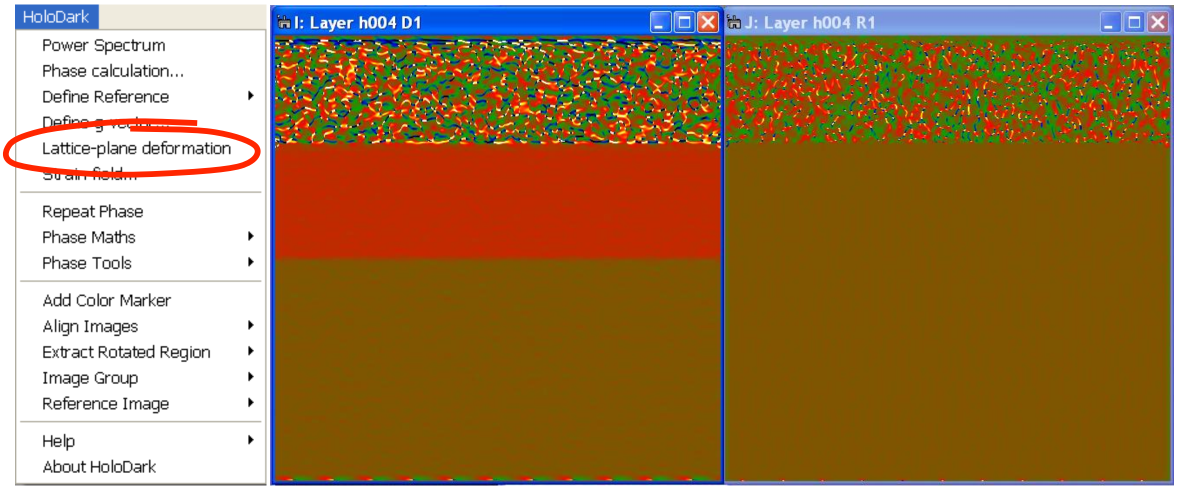


The arrow is a useful check to ensure that the correct direction has been chosen for the g-vector. You can see that the g-vector is indeed in the [001] growth direction.

Lattice-plane deformation

Now all is set to calculate the deformation of the (004) lattice planes from the phase of the dark-field hologram. The results concern the change in the spacing of the (004) lattice planes, with respect to the reference, and can be interpreted as the strain component, ε, in the [001] direction. The analysis will also give in-plane orientation of these lattice planes but beware: rotation can be due to the rigid-body of the whole crystal and/or shear. This is why we call it "lattice-plane deformation" to distinguish from the full 2D strain tensor determined later.

Select the phase image, and use the **HoloDark** command **Lattice-plane deformation**:

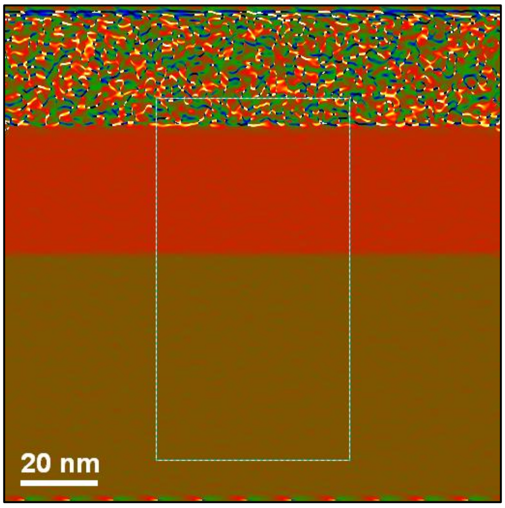


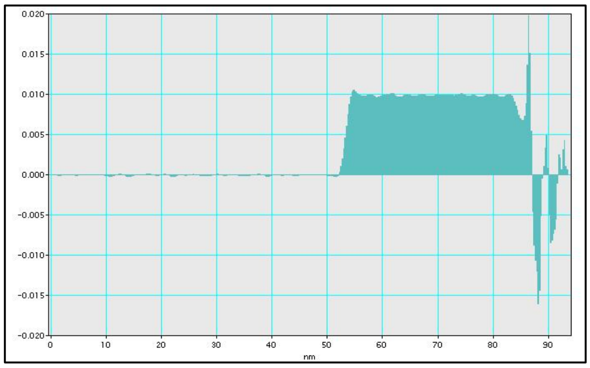
The first image (labelled D1) shows the change in lattice spacing relative to the reference lattice in fractional units (i.e. 0.02 means 2% expansion). The paired image (labelled R1) shows the rotation of the lattice fringes with respect to the reference in degrees (in-plane rotation and positive anticlockwise). By default the minimum and maximum values are (±5% deformation and ±5° rotation).

Precision and Spatial Resolution

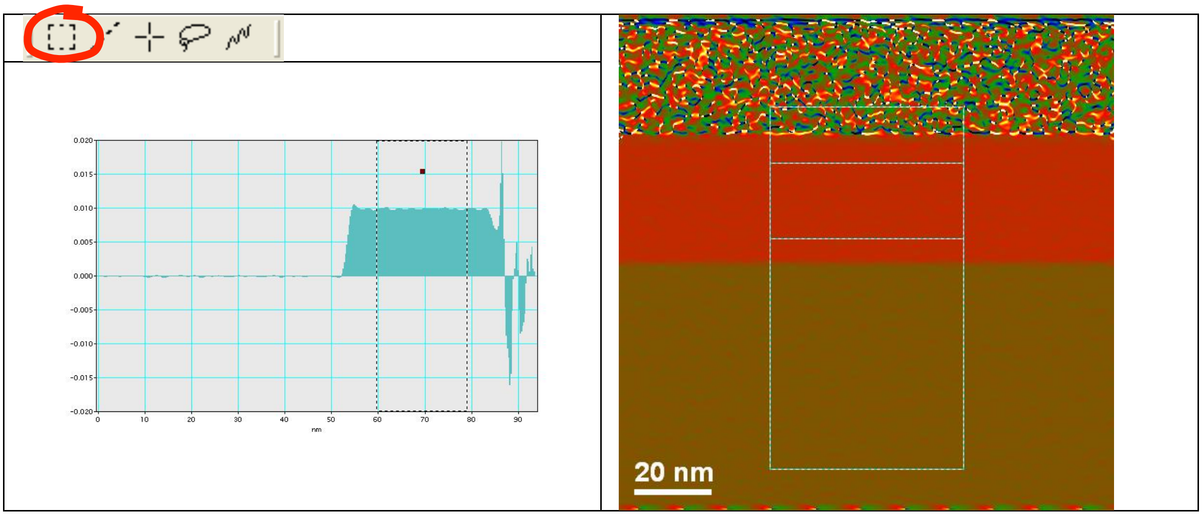
In this example, we can clearly see the strained layer and that the spacing of the lattice planes has changed with respect to the substrate (D1), whilst at the same time the lattice planes have the same orientation (R1). HoloDark is, however, much more than just a visualisation tool. Deformation can be measured using the profile tools and statistical tools in specified areas.

By choosing the DM **profiling tool**  , the (004) lattice parameter change can be visualised:



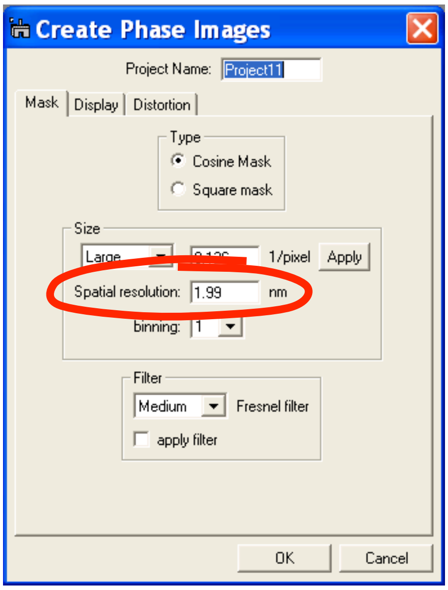


The deformation in the reference area of the substrate is zero as it should be. In the stained layer the change in the lattice parameter is 1%. To measure the value accurately, the DM **ROI** tool can be used on the profile with the useful feature that the region selected is shown on the deformation image at the same time. Now use the DM **Analysis…Statistics…Mean and Std. Dev**. The result gives the average value and an estimate of the error (the standard deviation).



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.

The *spatial resolution* depends on the mask size used in the analysis:



Technical note: We also provide the radius of the FFT mask, κ in pixels^{-1}, which gives a spatial resolution of 1/κ in pixels. Changing the mask size will change the spatial resolution (updated automatically).

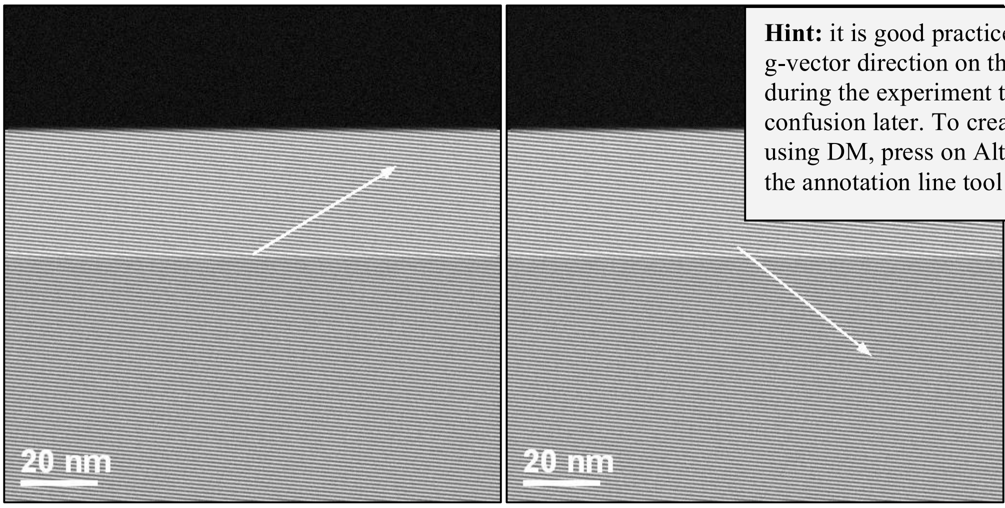
Hint: this is a handy way to know the holographic fringe spacing: with a Large mask size, the Spatial Resolution is exactly $2d_c$.

Repeat the whole example with a Small mask. Notice that the precision has increased for the deformation measurements but that the interface between the substrate and the layer appears wider in the line profile. This is an essential feature of local measurements, precision is inversely related to spatial resolution.

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

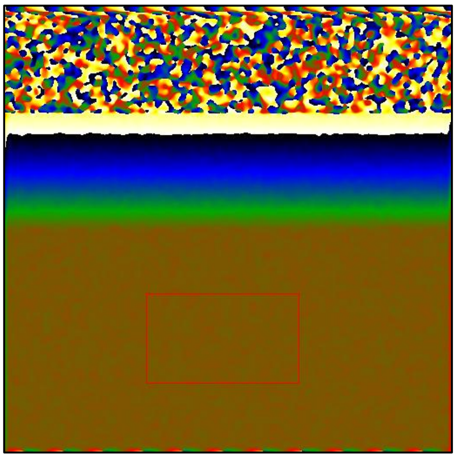
Determining strain tensors

In order to measure 2D strain tensors, dark-field holograms are required from two distinct and non-colinear g-vectors. Open the holograms “Thin layer h111” and “Thin layer h11-1”:

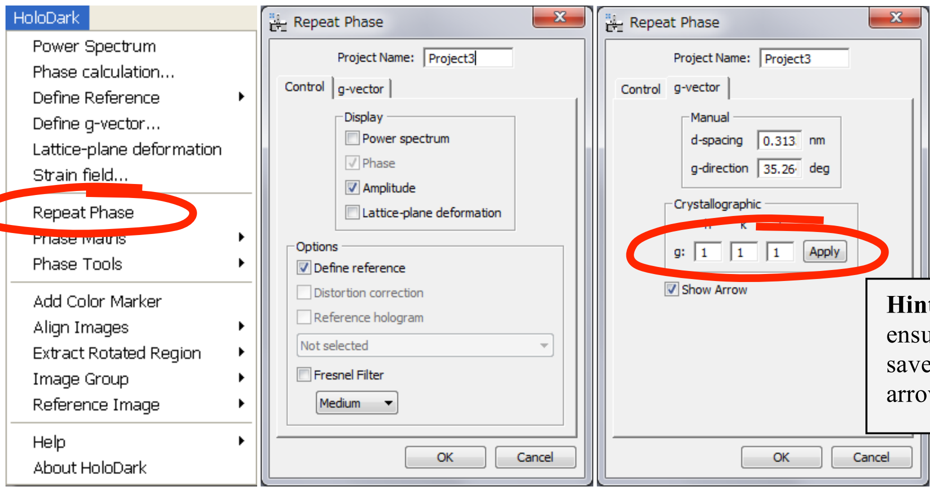


Hint: it is good practice to mark the g-vector direction on the hologram, during the experiment to avoid confusion later. To create an arrow using DM, press on Alt when using the annotation line tool (/).

As the names indicate, they were taken with the (111) and (11-1) g-vectors. First calculate the (111) phase image, including defining the reference area and g-vectors:

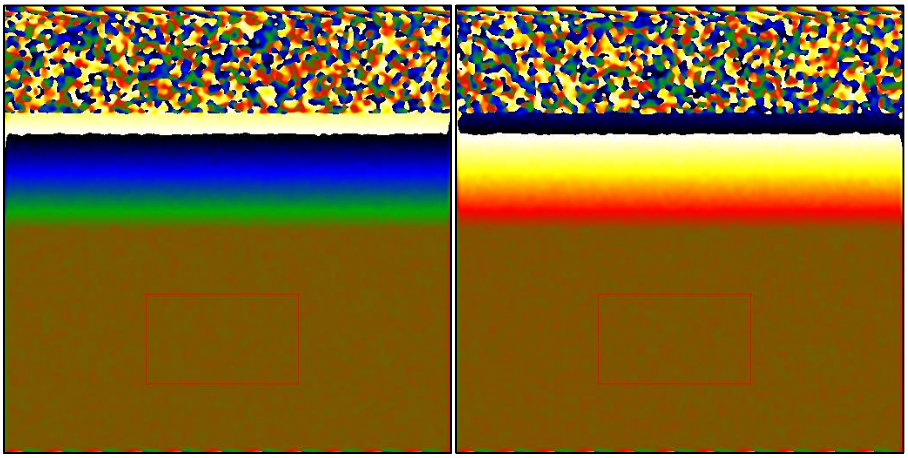


To create the (11-1) phase image, you might like trying the **HoloDark** command **Repeat Phase**. Select the “Thin layer h11-1” hologram image and choose **Repeat Phase** command:

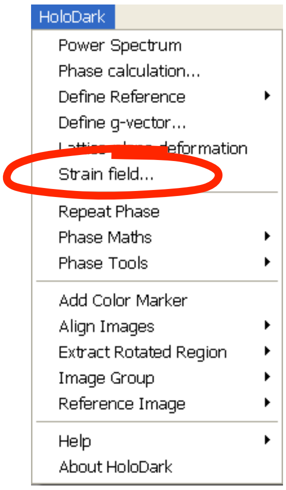


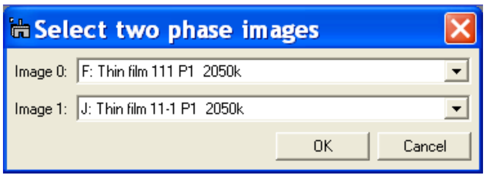
Hint: use **Apply** to ensure changes are saved and watch the arrow on the hologram.

All that needs changing is the g-vector indices to (1 1 -1) in the **g-vector** tab. Ticking the option **Define reference** is also useful, to ensure that identical reference areas are used on both images. The result, placed next to the (111) phase image, should be the following:

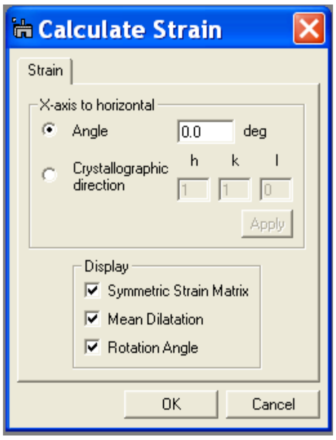


Now it is possible to calculate the 2D-strain tensor using **Strain field…**:

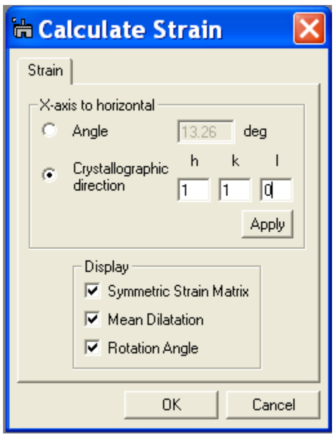




Hint: before choosing **Strain field…** click on the two phase images successively. They will then be proposed automatically as the two images 0 and 1.

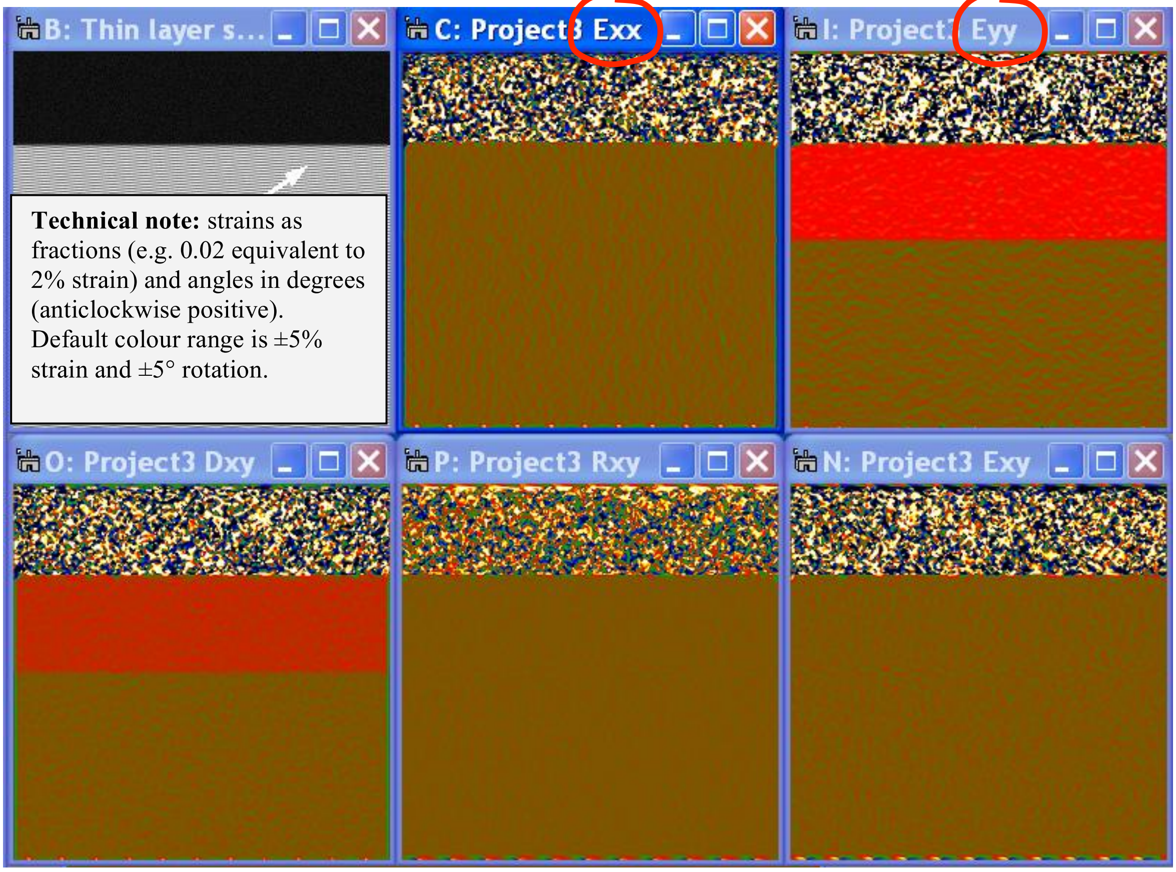


The **Calculate Strain** menu asks for a number of details, notably the definition of the *x-axis*. In this case, a natural choice is parallel to the interface i.e. at 0° to the image horizontal (as shown). Indeed, you may define the *x-axis* in any direction – HoloDark will carry out the mathematics – notably with respect to the crystallographic axes. Click on the **Crystallographic direction** and input [110] direction. Indeed, this is the default way of defining angles:



Hint: press Apply and you will see the Angle up-dated to zero.

With all the options ticked, the following group of images should appear:

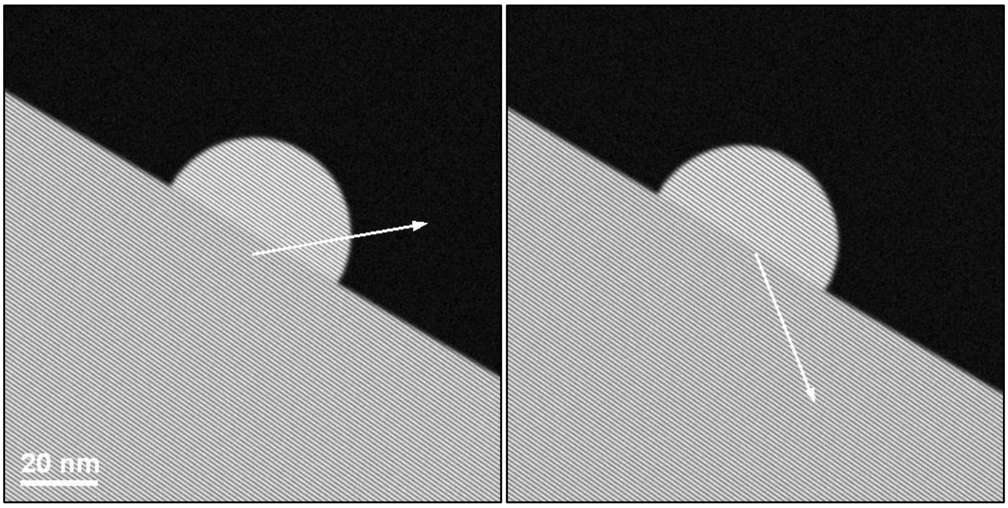


The lattice deformation in the x-direction, ε_{xx} (labelled Exx), is zero. This means that the layer has taken the same lattice parameter as the substrate parallel to the interface. You should find that the deformation in the y-direction, ε_{yy} (labelled Eyy), is identical to the deformation determined from the (004) diffracted beam, also in the y-direction. Indeed, measurements taken with different g-vectors should be consistent! The rigid-body rotation, ω_{xy} (labelled Rxy), and the shear, ε_{xy} (labelled Exy), are both zero indicating perfect epitaxy of the layer. Finally, the mean dilatation, Δ_{xy} is just the average of ε_{xx} and ε_{yy}. See the **Appendix** for the full definitions.

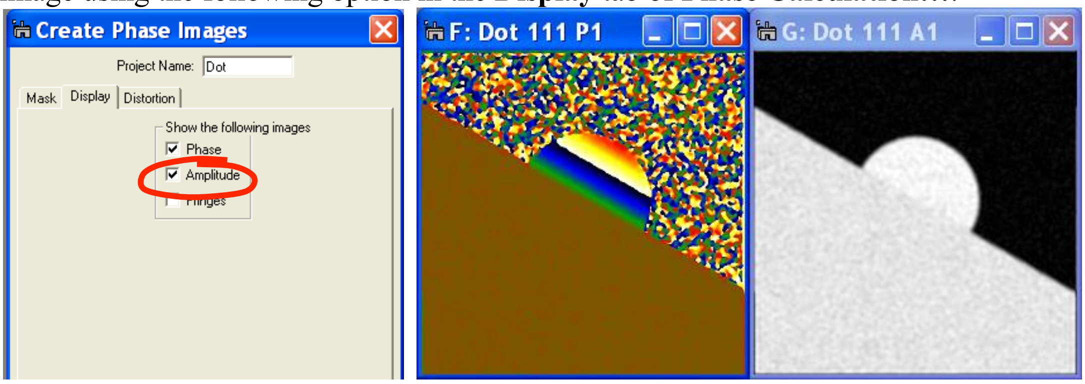
This is the final result of HoloDark strain analysis: the complete in-plane 2D strain tensor. Now we will investigate more realistic examples.

Image alignment

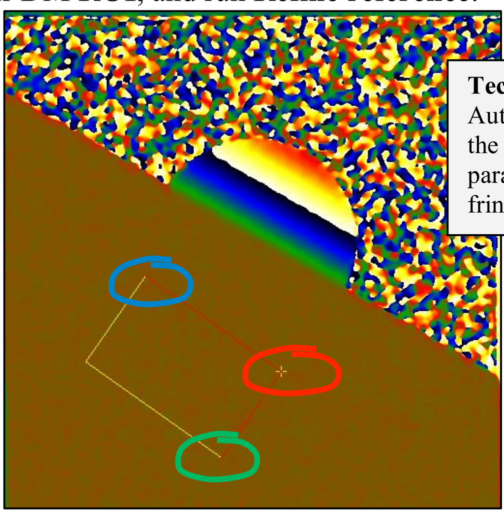
Open the two holograms “Dot h 111” and “Dot h 11-1” of a strained nanocrystal on a silicon substrate:



The zone-axis is [1-10] as before and the surface normal [001]. Now calculate the (111) phase image using the following option in the **Display** tab of **Phase Calculation…**:



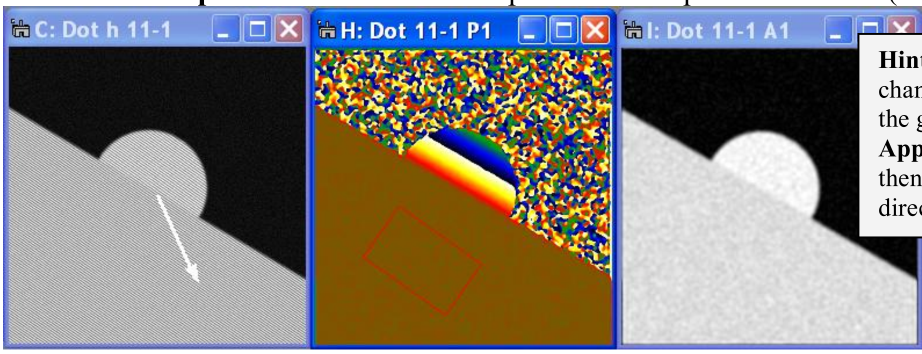
The amplitude image (A1) shows the local contrast of the holographic fringes, which is slightly higher in the nanocrystal and zero in the vacuum. This image will be useful for alignment purposes. Now choose the following options in the **Refine reference… Setup** menu, place a rectangular DM **ROI**, and run **Refine reference**:



Technical note: the Automatic option means that the rotatable ROI is oriented parallel to the holographic fringes.

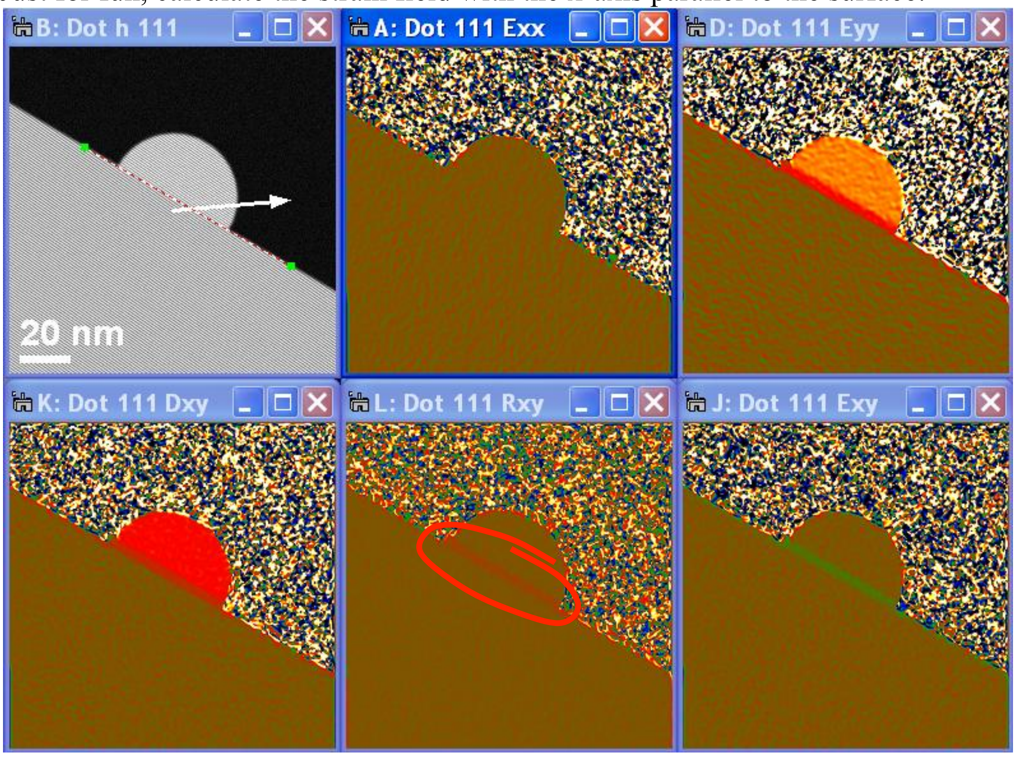
The ROI is rotatable (use the top-right corner, circled in red, to rotate) and the size can be changed lengthwise (bottom-right, in green) and heightwise (top-left, in blue). The whole object can be grabbed and displaced by clicking anyway within the ROI. The most logical choice is to rotate the ROI parallel to the specimen surface.

Now use the **Repeat Phase** command to produce the equivalent for the (11-1) hologram:



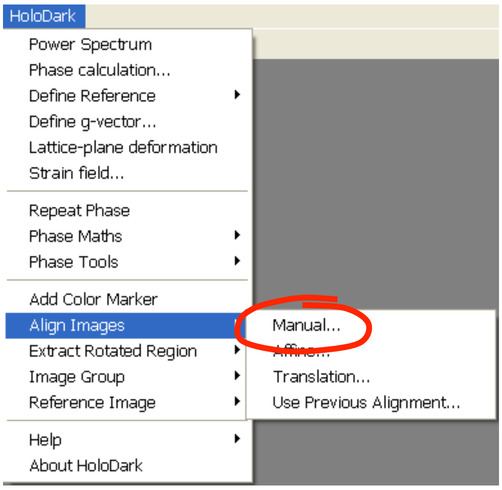
Hint: remember to change the indices for the g-vector and press **Apply**. The arrow will then show the correct direction.

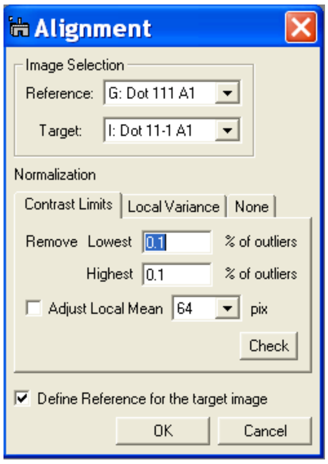
Just for fun, calculate the strain field with the x-axis parallel to the surface:



Notice that there seems to be a strange interface layer between the substrate and the nanocrystal containing lattice rotation and shear. Indeed, on closer inspection, the images seem somewhat blurred at the edges. The reason is that the two holograms are not perfectly aligned. During experiments the specimen will drift and changing from one diffraction vector to another introduces image shifts. For experimental holograms this will always be the case. This is why we have developed alignment routines for HoloDark.

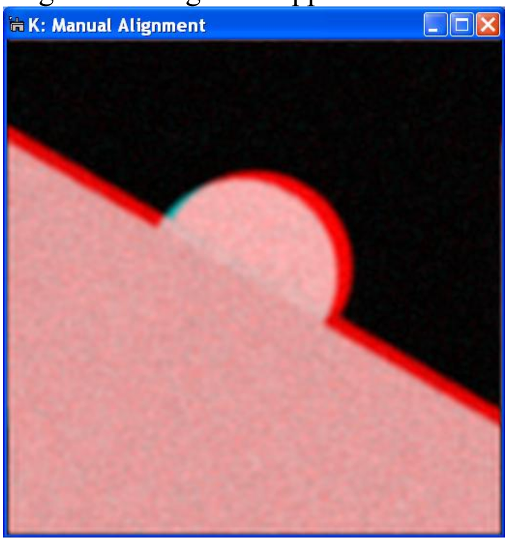
In most cases, it is easier to carry out alignements based on the amplitude images. Select the two amplitude images successively and run the **Align images…** command.

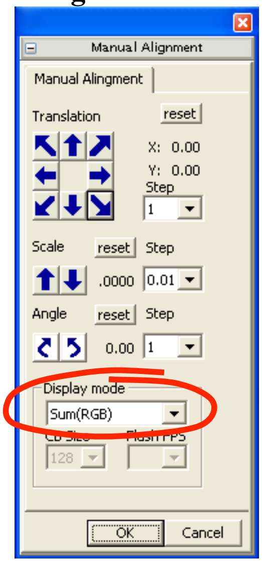




Technical note: the option **Define Reference** ensures that identical reference areas are used on the two aligned phase images.

In the **Image Selection**, the **Target** image is going to be shifted to be aligned with the **Reference** image. In our case, the two amplitude images have been chosen. Do not worry about the other options for the moment, and click on OK. Two things will happen, a Manual Alignment image will appear and a **Manual Alignment** control box:

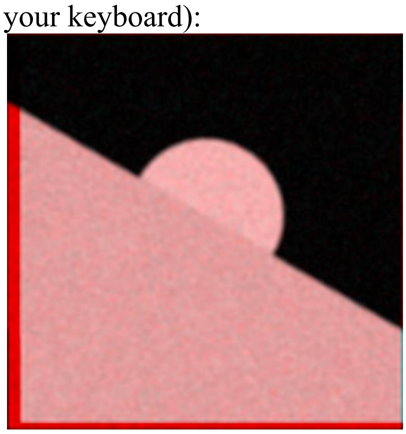




Technical note: for completeness, corrections can be made for changes in magnification (Scale) and image rotation (Angle). However, for DFEH these are rarely necessary.

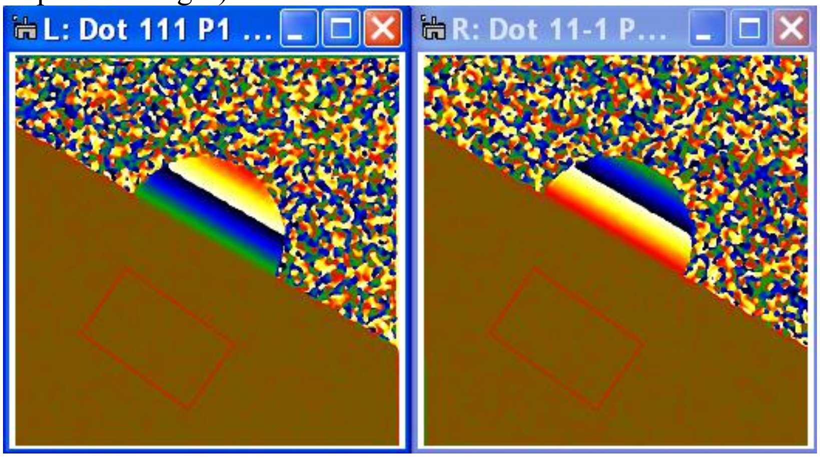
Hint: in this case, you do not need sub-pixel alignment so leave the **Step** size as it is.

Different **Display modes** have been included as everyone has their favorite (e.g. **Difference**). For the **Sum (RGB)** option, both amplitude images are shown on top of each other, one in red (*Reference*) the other in cyan (*Target*). You can clearly see that the images are misaligned. Click on the **Translation** arrows to find the best alignment (you can also use the arrows on your keyboard):

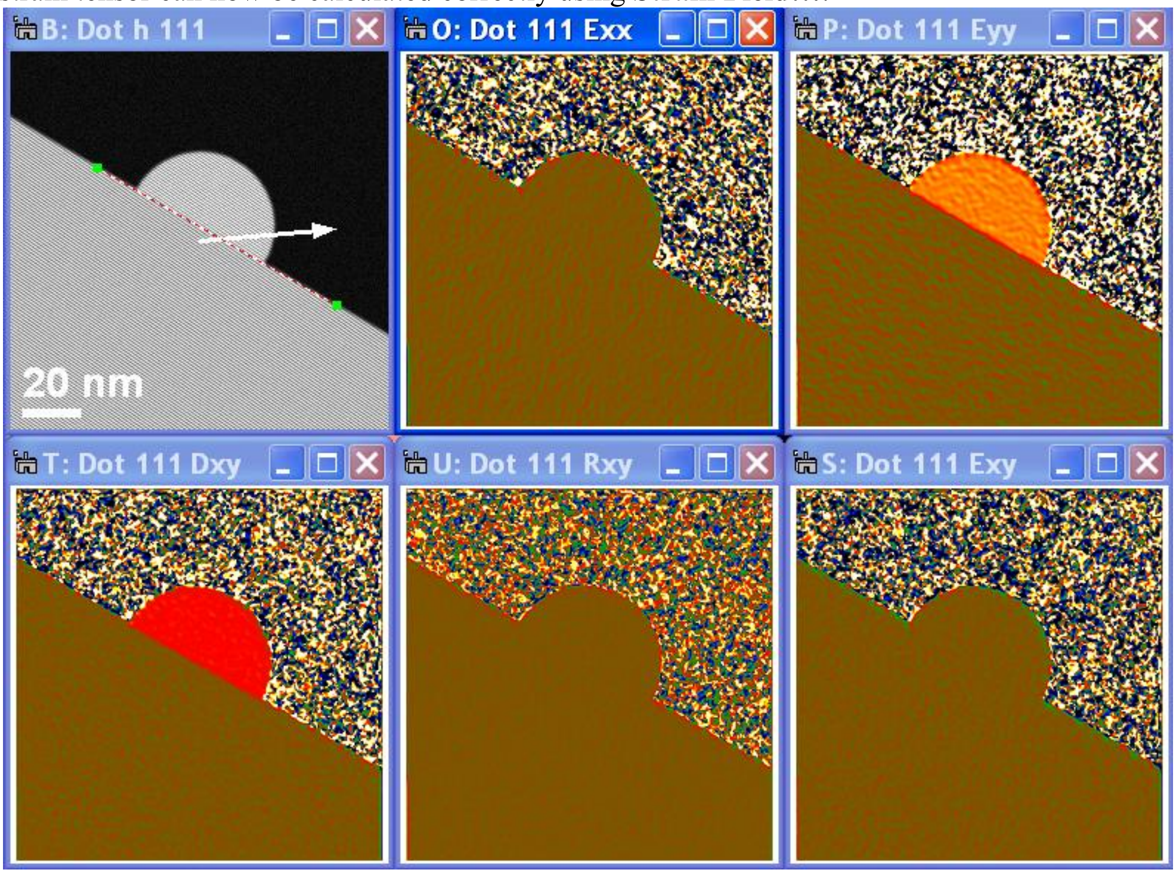


Hint: if you ever get "lost in alignment", press on the **reset** buttons to return to starting values.

Once satisfied, click on OK and HoloDark will display the aligned phase images (and amplitude images):



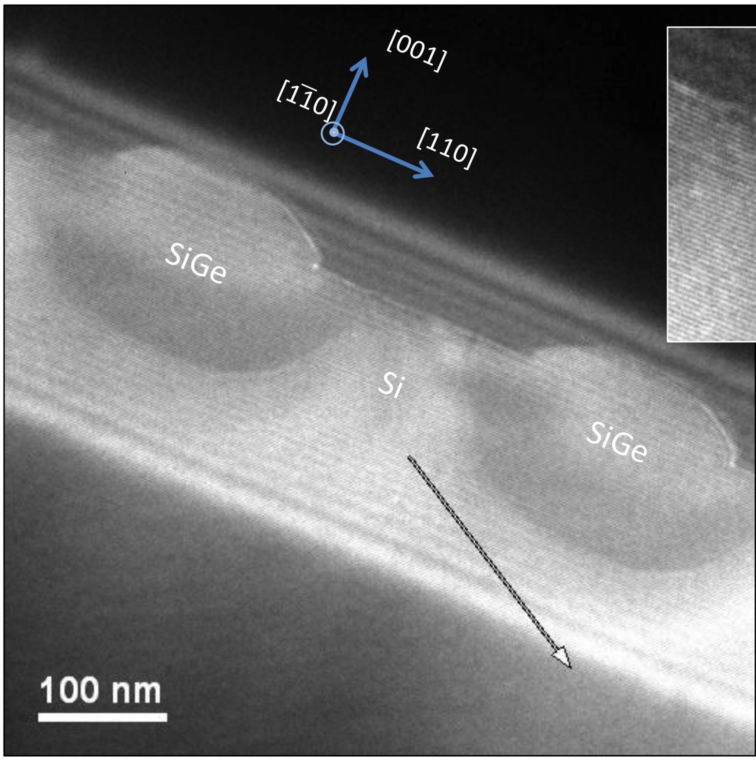
The images have been cropped to show only the area common to both holograms. The 2D strain tensor can now be calculated correctly using **Strain Field…**:

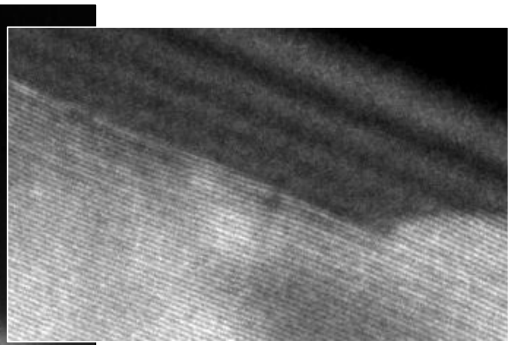


Compare these images with the previous set and you will see the improvement.

Experimental Example

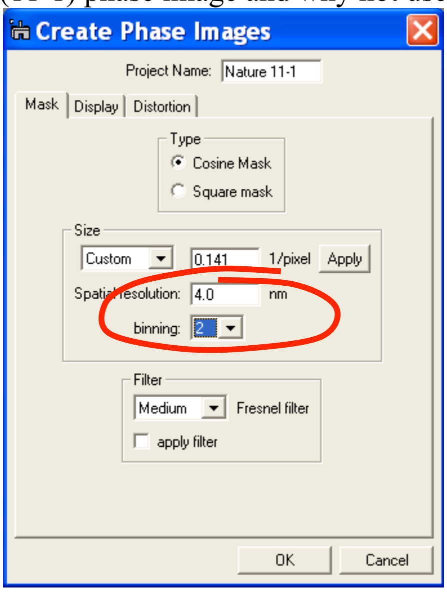
We are now ready to attack a real experimental example that will introduce the final set of HoloDark tools and corrections. It concerns the strained-silicon MOSFET device analysed in the original DFEH paper *M.J. Hÿtch et al., Nature 453 (2008) 1086*. Open the (11-1) hologram “Nature h 11-1”:





Technical note: the fringes in the vacuum are Fresnel fringes from the biprism. Note that the holographic fringes are not present in the vacuum.

Real holograms have Fresnel fringes and do not cover the whole field of view. Calculate the (11-1) phase image and why not use the *Binning* option:

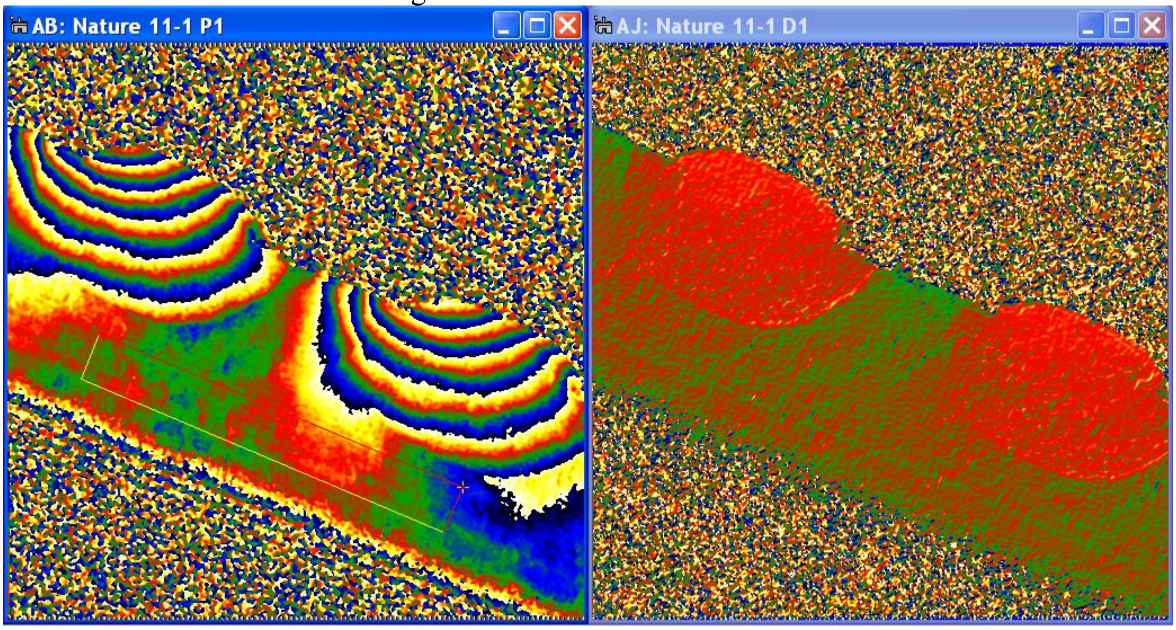


Technical note: the binning is necessarily at least 4 to use the Square mask.

Hint: fix the spatial resolution to standardized numbers so that results can be readily compared between experiments. Use the Large mask as a guide and then round upwards.

Binning means that the phase images are reduced in size, by the binning factor, compared with the original image. This speeds up processing and economises space. No information is lost because the masking eliminates most of Fourier space anyway.

Define the reference and the g-vector as usual and calculate the lattice-plane deformation. You should arrive at the following result:

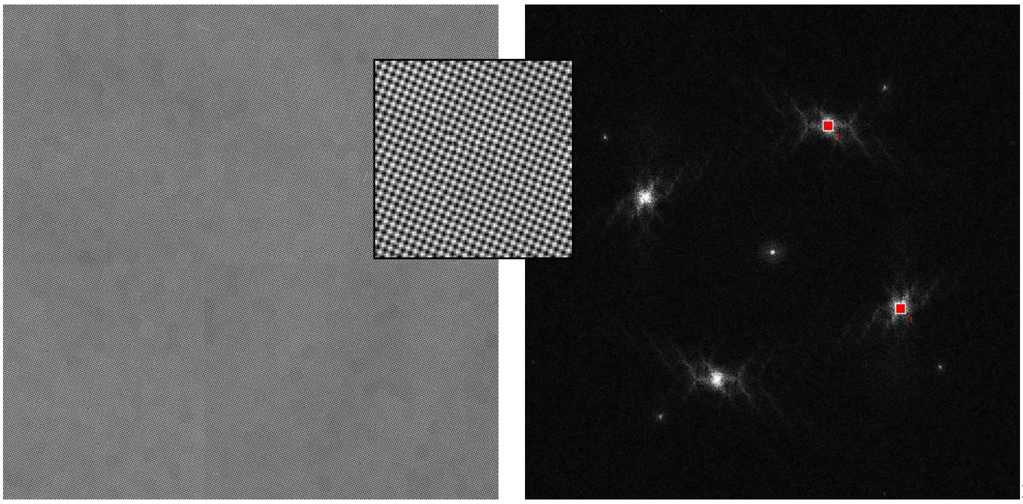


Notice the high-frequency variations in the deformation map which even look as if they are on a hexagonal network. These artefacts are due to the geometric distortions of the CCD camera.

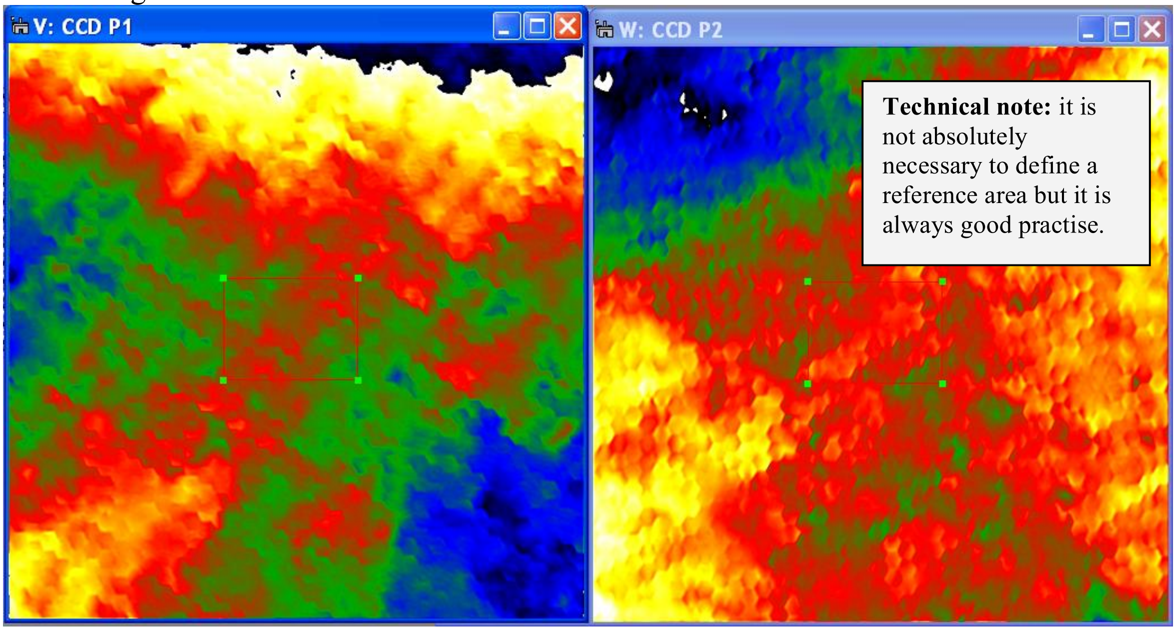
Geometric distortion correction

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 them 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 of perfectly periodic fringes, such as a hologram in the vacuum covering the whole field of view.

In order to correct for distortions, you need to set up a **Reference Image**. Open the image "Nature CCD" and calculate the *Power Spectrum*.


:

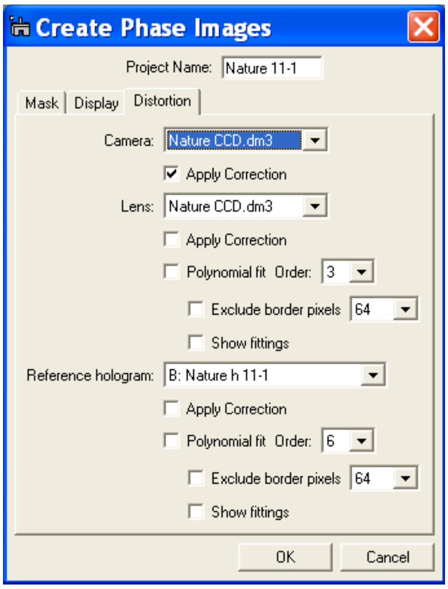
This special image has been kindly supplied by Gatan (courtesy of Paul Mooney). Calculate a pair of phase images by selecting two spots in the *Power Spectrum*. In principle the mask size and binning do not matter:



Technical note: it is not absolutely necessary to define a reference area but it is always 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 *HoloDark Reference* is created in *My Images* folder but you can place your reference images anywhere. Give the file a name, say "Nature CCD", and click OK. The program will save the Nature CCD image with the necessary information for later use.

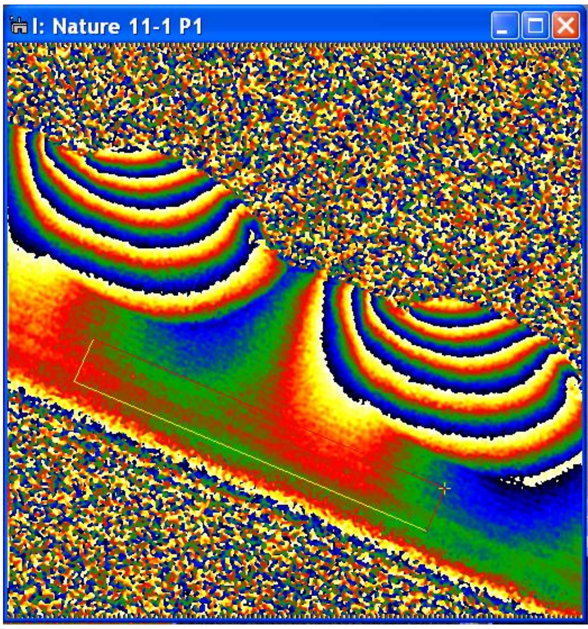
Redo a **Phase Calculation…** for the (11-1) hologram. At the menu stage, click on the **Distortion** tab. It should look something like this:

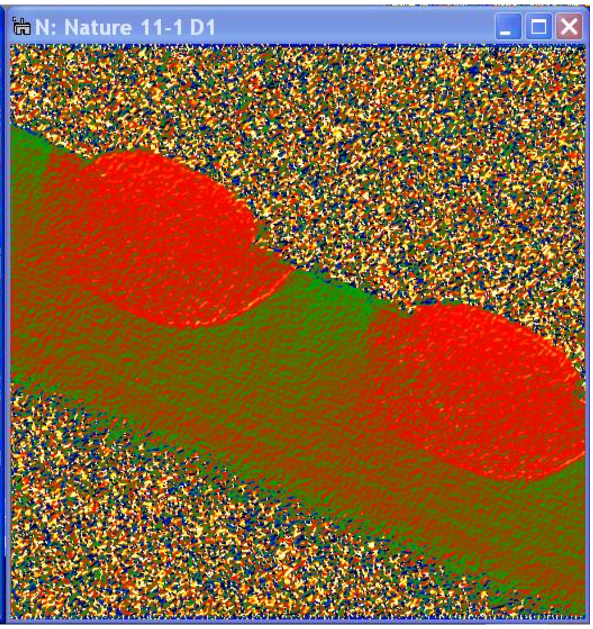


Technical note: lens distortions can be corrected with a suitable reference image. The distortions are smoothly varying and can be fitted with a low-order polynomial.

The required **Reference Image** can be chosen using the scroll down menu **Camera** and/or **Lens**. For example, you could have a list **Reference Images** for different cameras on different microscopes. When you have selected the Nature CCD, tick **Apply Correction** and click **OK**.

The phase images will be corrected automatically and, after using **Define Reference**, will have a more uniform appearance:

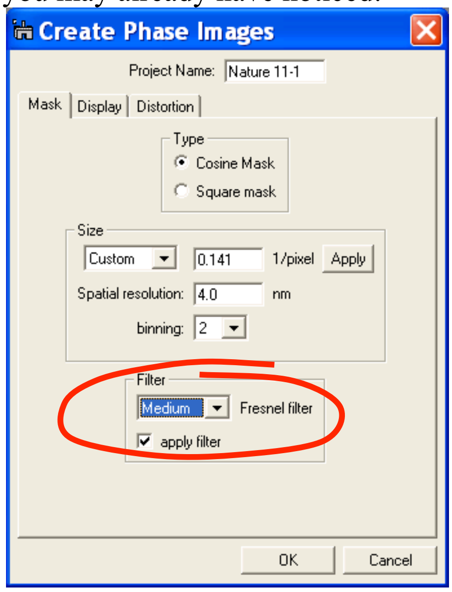




You only need to define the *Reference Image* once. From now on, it will be available in the **Phase Calculation...Distortion** tab. If you wish to delete it, just use **Reference Image...Delete….**

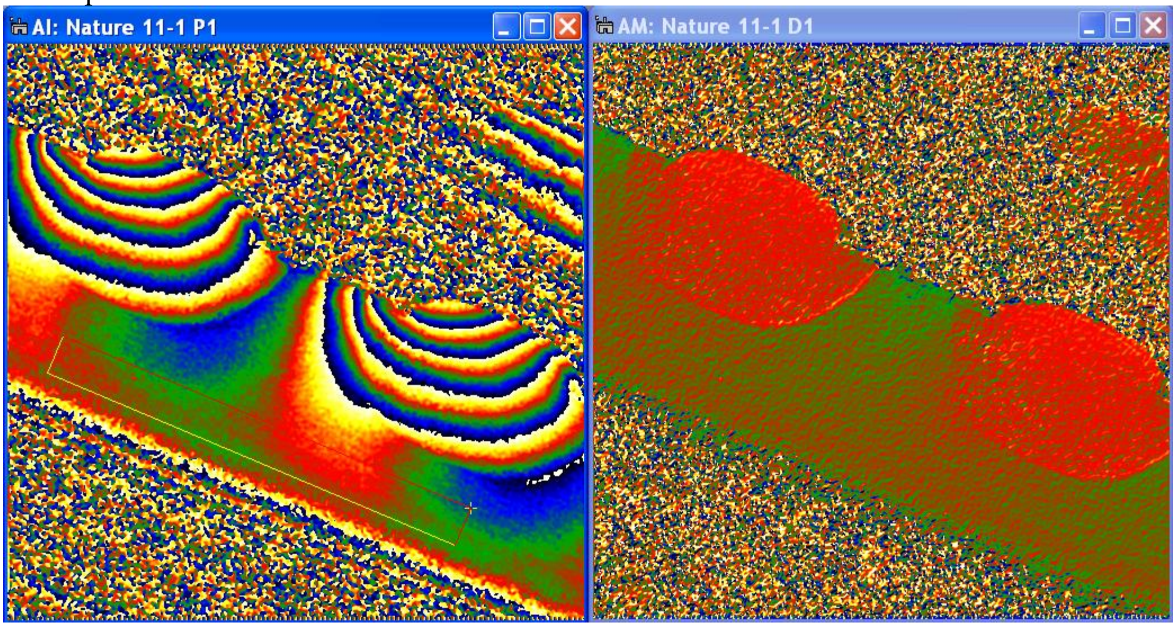
Fresnel fringes

In the substrate, the deformation is still not completely uniform. Some long-range variations are real but the horizontal lines are due to another effect – the Frensel fringes from the biprism. No ideal solution exists to deal with these artefacts (except avoiding them in the first place by using multiple biprisms). However, we have included in HoloDark a simple Fourier space filter to reduce their effect. Recalculate the phase image using the **Fresnel Filter** option which you may already have noticed:

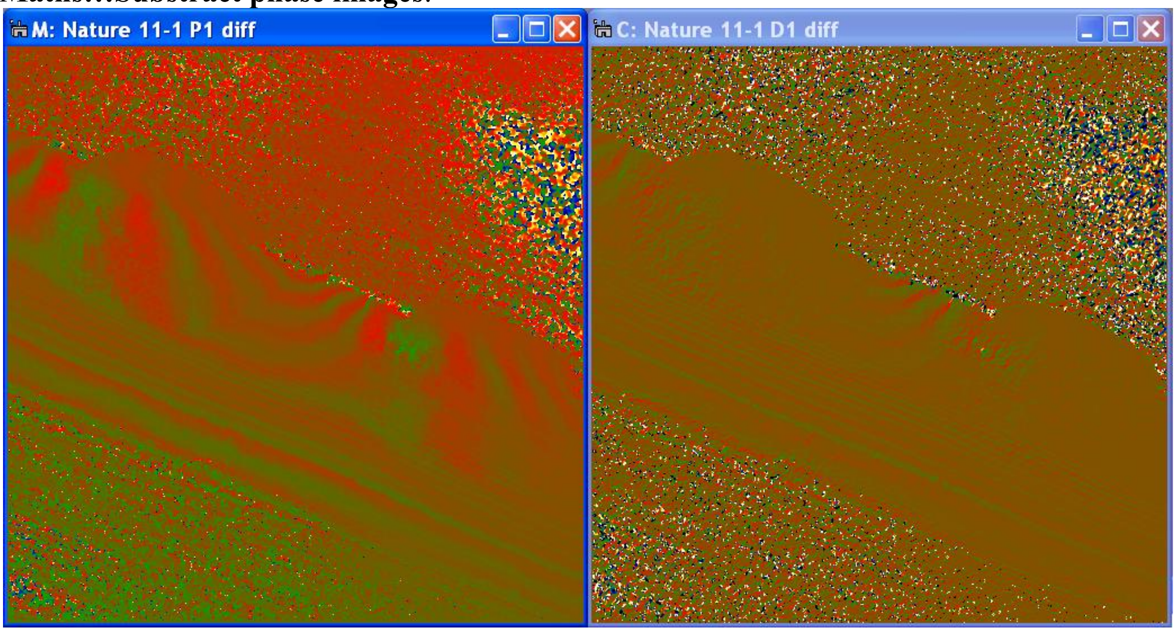


Technical note: the filter just masks out a strip in Fourier space between the origin and the side band. The *Weak*, *Medium* and *Strong* indicate how close the mask gets to the side band spot. As usual, the weaker the filter the better and no filter is best of all!

Choose the *Medium* filter and calculate the phase (with distortion correction) followed by the lattice-plane deformation:



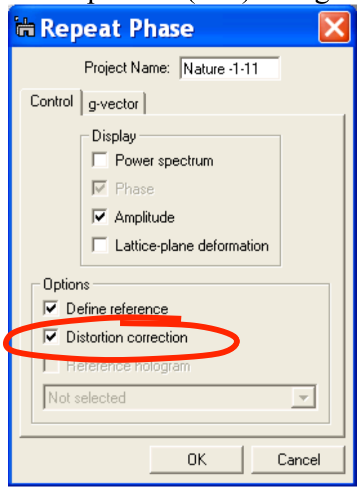
Notice how the phase and the deformation are much smoother in the substrate. As a note of warning, however, notice also the patch of contrast which has appeared in the vacuum! Filters always have such non-local effects. The best test is to subtract the original from the filtered image to assess whether the results seem reasonable. For the phase image use **Phase Maths…Substract phase images**:



In this case, you might want to worry about the moiré like effects created by the filter for quantitative measurements of strains in certain regions.

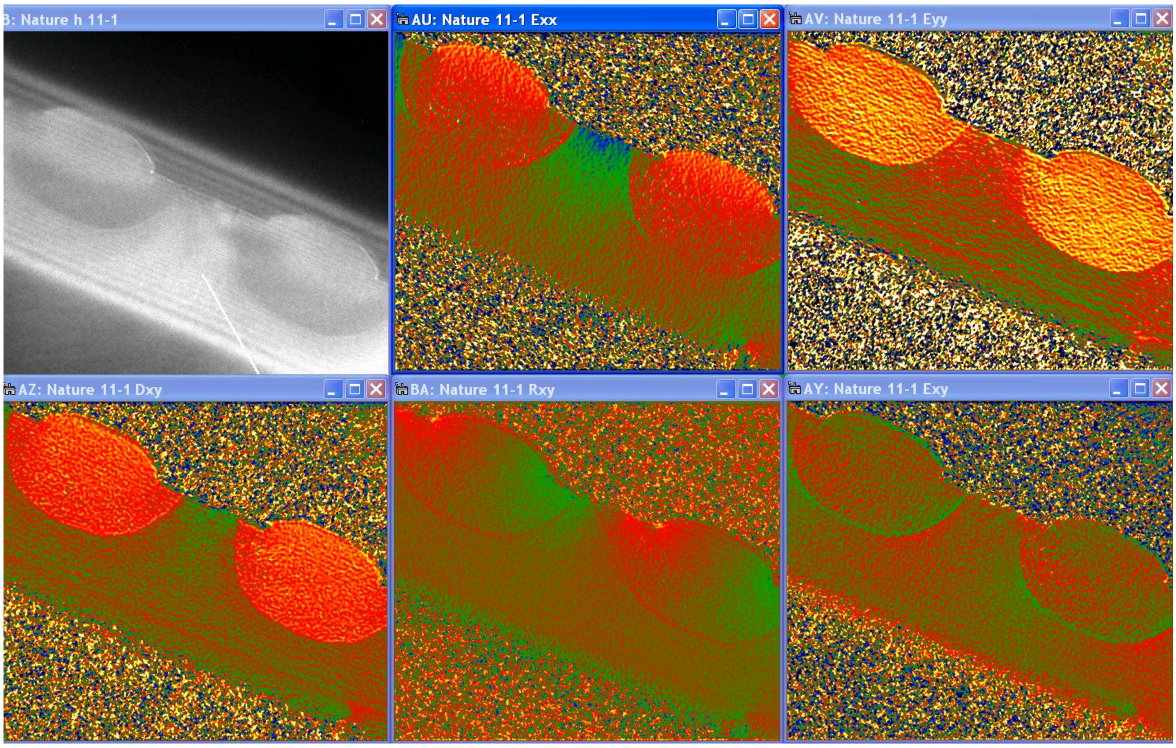
Ultimate analysis

Now open the (111) hologram and calculate the phase image using **Repeat Phase:**

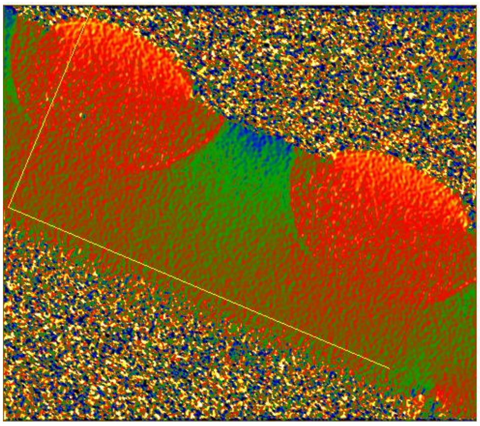


> **Technical note:** the **Distortion correction** box is no longer greyed out as the previous phase calculation made use of it.

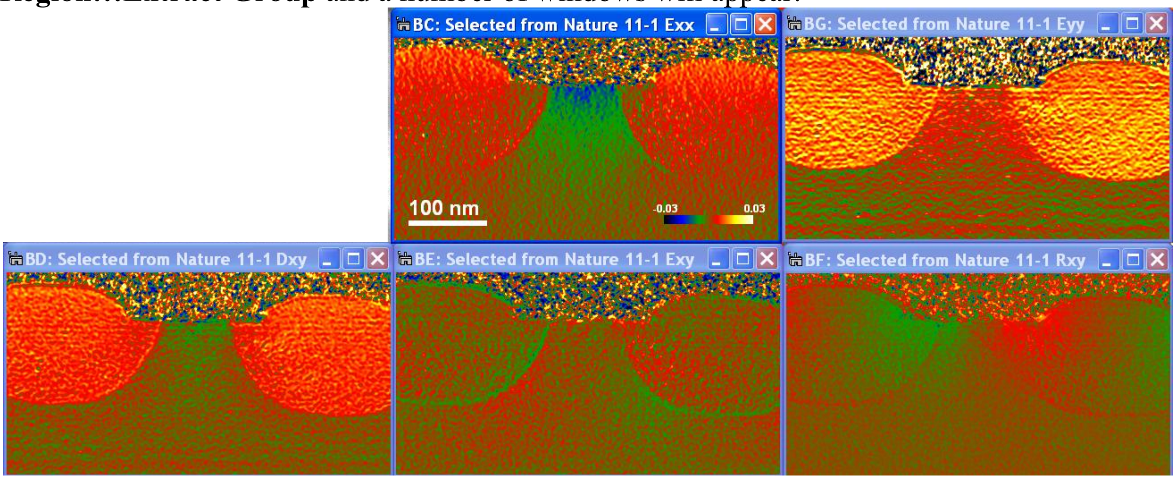
Follow through the analysis, including g-vector definition and image alignment, to produce the 2D strain tensor:



Before finishing, there is just one icing on the cake. Mark a DM rectangular **ROI** on the Exx image and use the **Extract Rotated Region…Define** function:



Rotate and adjust the rotatable ROI shape and size. Now use **Extract Rotated Region…Extract Group** and a number of windows will appear:



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

This marks the end of the tutorial. Now it is time to enjoy analyzing your own data with HoloDark.

Appendixes

A: Important phase relations

Phase and displacement:

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

2D displacement and phase:

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

Phase gradient and reciprocal lattice deviation :

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

Strain tensor for small deformations:

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

Mean dilatation :

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

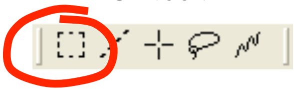
Rotation (in radians and anti-clockwise positive):

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

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

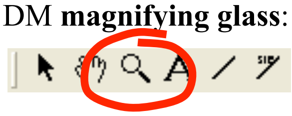
B: Useful DigitalMicrograph commands

DM **ROI tool**:



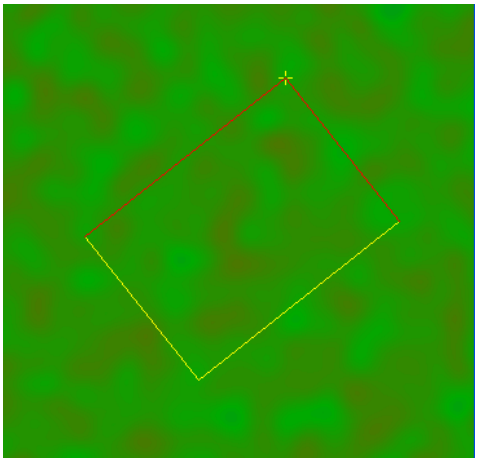
Hint: to select a square area, hold down SHIFT.
To select powers of two, hold down SHIFT-ALT.

DM **magnifying glass**:



Hint: to demagnify, press ALT.

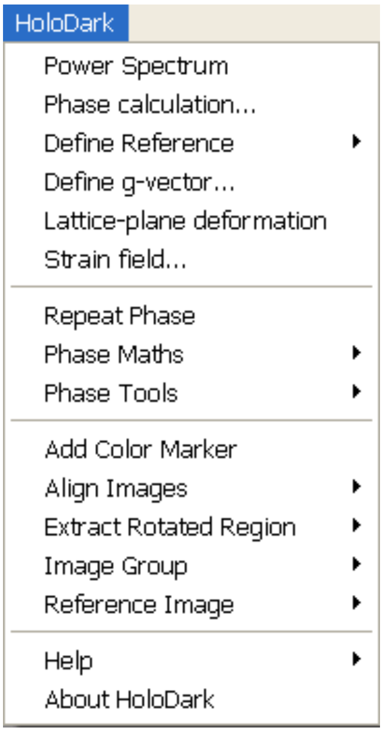
C: Rotatable ROI



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 HoloDark Main Menu



The commands in the HoloDark menu are described below.

Command	Description
Power Spectrum	First step in the HoloDark procedure. Calculates and displays the Fourier transform of the front most hologram image. The centre of a side-band is then selected in the image of the Fourier transform (called Power Spectrum) using the mouse tool.
Phase calculation…	Second step in the HoloDark procedure. Calculates phase image for the side-band selected in the Power Spectrum (see options).
Define Reference (see sub menus)	Menu concerning the reference region and third step in the HoloDark procedure. You can use this command to refine the reference region simultaneously on two images after alignment.
Define g-vector…	Defines the value of the diffraction vector (g-vector) in image coordinates, forth step of the HoloDark procedure.
Lattice-plane deformation	Calculates the deformation of lattice planes from the front-most phase image. Displays variation in planar

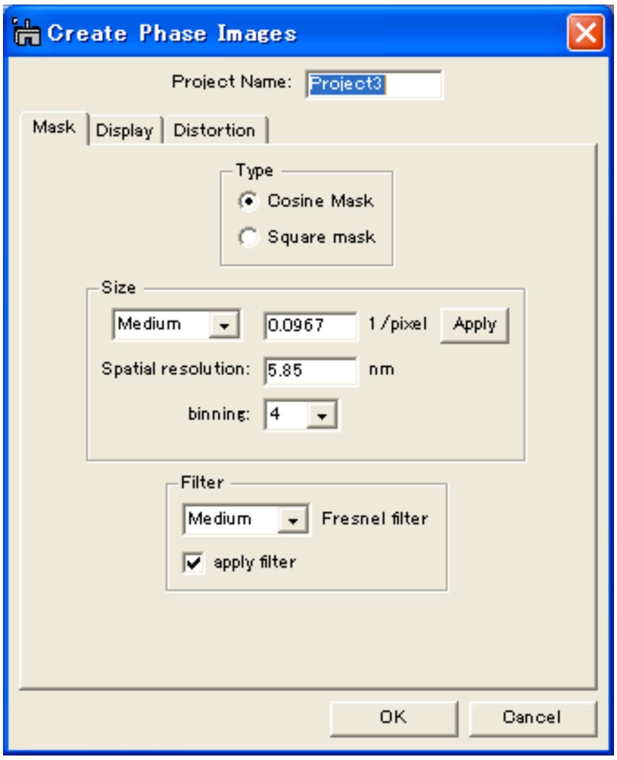
	spacing (with respect to reference) and orientation (in degrees, anticlockwise positive).
Strain field…	Calculates the two dimensional deformation tensor. Asks for two phase images and options (see below).
Repeat Phase	Allows phase images and other output to be generated directly from the front-most hologram image, exactly as for a previous calculation.
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.)
Align Images (see sub menus)	Allows two phase images from different holograms to be aligned. Corresponding amplitude images will usually be use to find alignment conditions.
Extract Rotated Region (see sub menus)	Extracts a region(s) of interest from the processed image(s). The region to be extracted can be arbitrarily rotated, and then the long edge direction will be rotated to horizontal. The final display can be further rotated by 90, 180 or 270 degrees.
Image Group (see sub menus)	Menu to close or save groups of images that are related with each other, e.g. strain maps.
Reference Images (see sub menus)	Menu to define reference images for distortion correction due to CCD cameras or projector lenses.

Phase Calculation
(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.

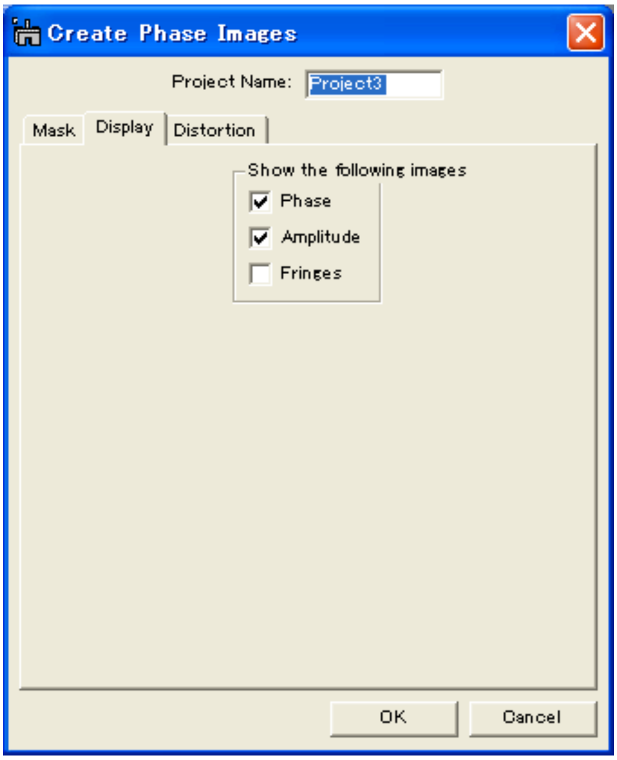
Mask Tab



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).
Square Mask	Square-shaped mask with a hard cut-off. Size

	corresponds to the distance from the centre to the edges (i.e. half the side length).
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.
Filter	Controls the filter to reduce effects from the Fresnel fringes.
Fresnel Filter	Defines the strength of the filter: weak (0.9), medium (0.95) and strong (0.98). The number indicates the fraction of the segment between centre-band and side-band which is removed by the mask.
Apply Filter	Tick to apply the Fresnel filter.

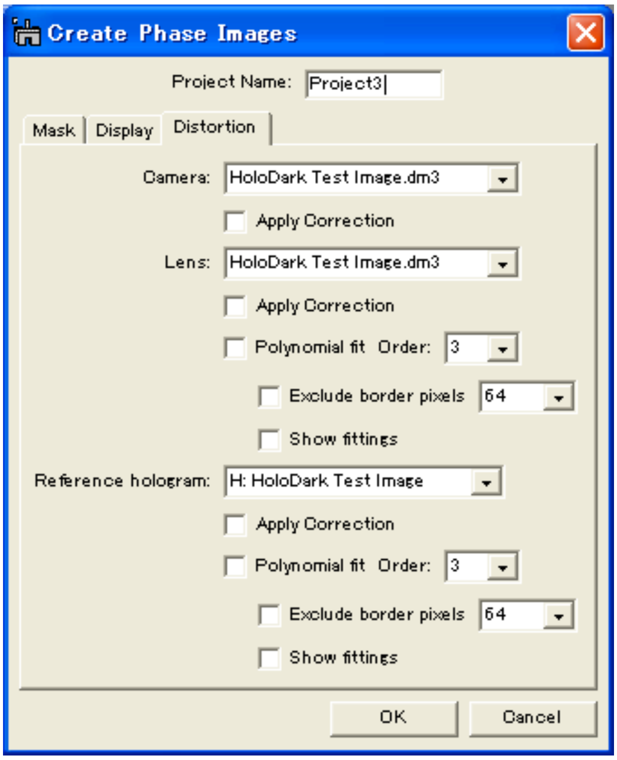
Display Tab



Component	Description
Display	Choice of images to be calculated and displayed.

Phase	Phase image from selected side-band.
Amplitude	Amplitude image from selected side-band.
Fringes	Image of the selected side-band 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).
Reference hologram	Selection of the reference hologram used for correcting distortions due to bi-prism.
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 (maximum 6).
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	Before running the command, an area needs to be selected by the DM rectangular ROI tool. The command defines this region as the reference lattice and adjusts phase images accordingly (see options). The rectangular ROI can be made rotatable (see Setup).
Setup…	Opens Setup dialog.

Setup Dialog

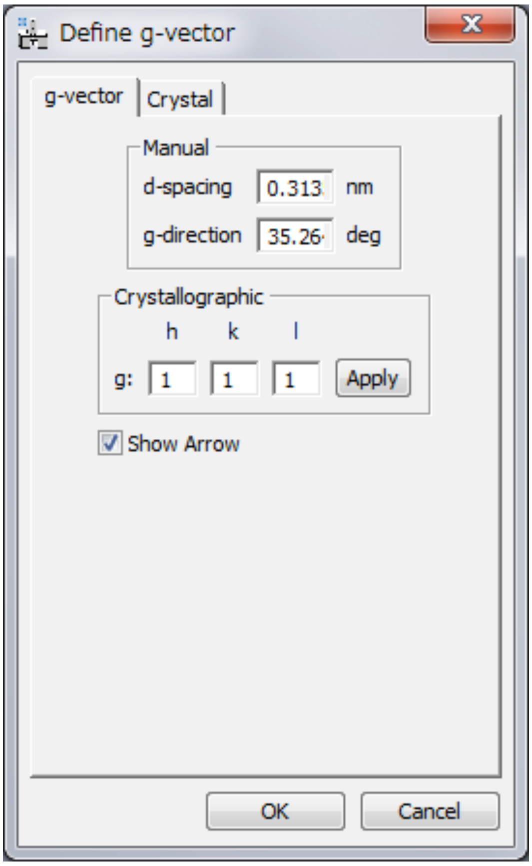
Option	Description
Automatic Update	Moving the reference area automatically updates the phase images and reference values.
Show qx,qy	Displays the values of the side-band center (qx, qy) in the DM Results window each time the reference area is updated.
Rotatable	Tick to make the rectangular ROI rotatable.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

Define g-vector
Define g-vector Dialog

The components of the dialog are described below.

Component	Description
g-vector Tab	For information about the components of the g-vector tab, see g-vector Tab below.
Crystal Tab	For information about the components of the Crystal tab, see Crystal Tab below.
OK	Closes the dialog and starts the image calculation according to the specified parameters.
Cancel	Closes the dialog without executing the command.

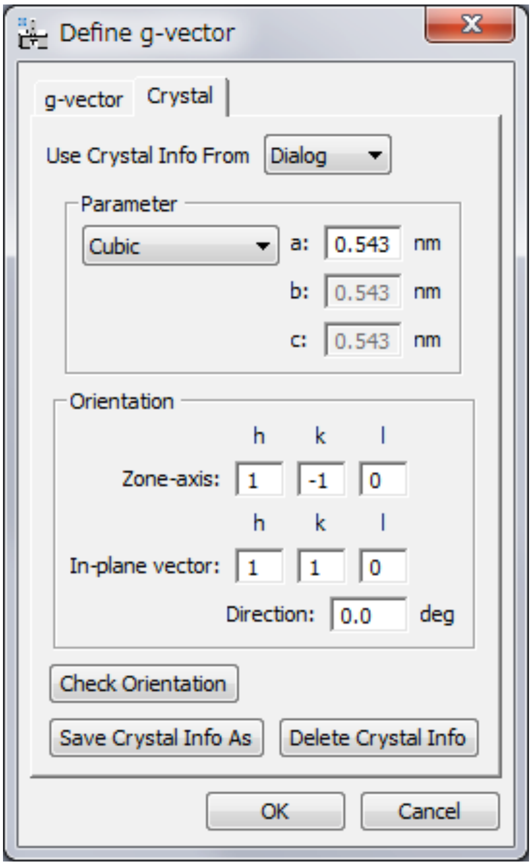
g-vector Tab



Option	Description
Manual	Manual setup for the diffraction vector (g-vector) used to obtain the hologram.
d-spacing	Planar spacing in nm corresponding to g-vector.
g-direction	Angle of g-vector with respect to the image horizontal (anticlockwise positive).
Crystallographic	Crystallographic setup for the g-vector used to obtain the hologram. Please make sure the *correct* crystal

	settings have been defined (see Crystal tab).
g (h k l)	Miller indices of the diffraction vector.
Apply	Confirms the crystallographic definition. On click, d-spacing and g-direction calculated and displayed (and see Show Arrow). This button becomes active, only when the Crystal settings have been defined.
Show Arrow	Tick so that on Apply, an arrow is shown on original hologram image in the direction of the g-vector.

Crystal Tab

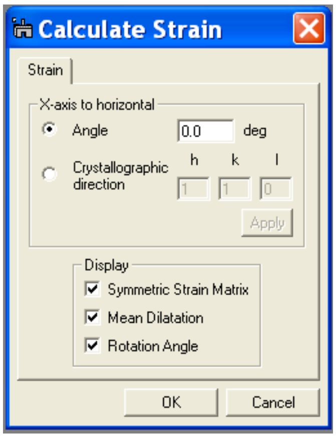


Option	Description
Use Crystal Info From	Selection of crystallographic information from the current dialog or the saved crystal Info.
Parameter	Defines a crystal system and a unit cell.
Crystal system	Selection of the crystal system from cubic, tetragonal or orthorhombic.
a, b, c	Lattice parameter in nm.
Orientation	Parameters to define crystal orientation with respect to hologram image.
Zone-axis	Miller indices of zone-axis normal to hologram plane in upward direction (i.e. opposite direction to incident beam).
In-plane vector	Miller indices of any reciprocal lattice vector within the

	plane of the hologram (not necessarily the diffraction vector).
Direction	Orientation of in-plane vector with respect to image horizontal (anticlockwise positive). Taken by default from a DM line ROI, if marked on original hologram image.
Check Orientation	Confirms new crystallographic parameters and orientation.
Save Crystal Info As	You can save the crystal information defined in the current dialog under the specified name.
Delete Crystal Info	Delete the saved crystal Info from the list.

Strain Field

(Calculate Strain Dialog)



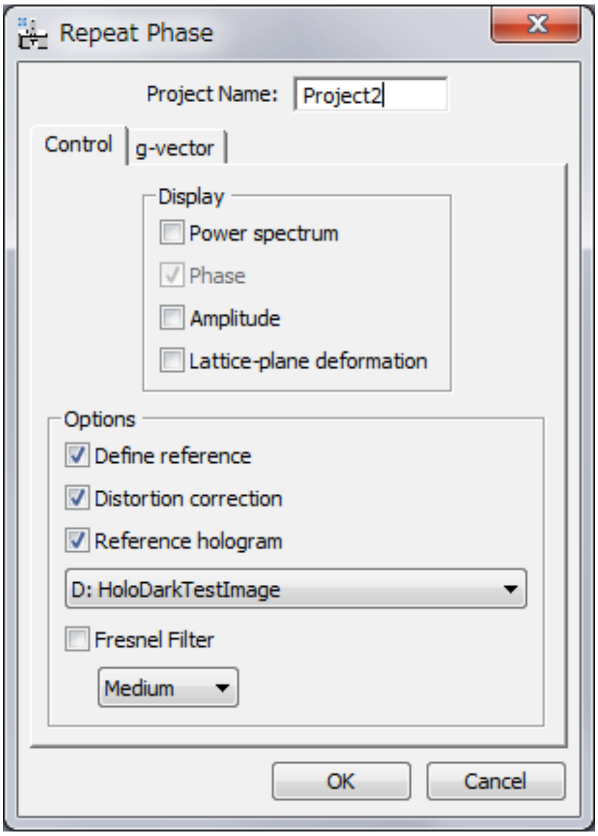
Component	Description
X-axis to horizontal	Defines the orientation of the x-axis used for calculating the strain tensor components. Angle defined from the image horizontal to the desired x-axis (in degrees, anticlockwise positive). The values used for the previous calculation will be shown.
Angle	Allows angle to be defined manually.
Crystallographic direction	Allows angle to be defined using crystallographic coordinate system (see define g-vector…Crystal tab). Miller indices of x-axis direction.
Apply	Confirms and applies the crystallographic definition (Manual Angle will be modified and displayed automatically).
Display	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.

Repeat Phase

The components of the dialog are described below.

Component	Description
Project Name	Allows a new project name to be defined.
Control Tab	For information about the components of the Control tab, see Control Tab below.
g-vector Tab	For information about the components of the g-vector tab, see g-vector Tab below.
OK	Closes the dialog and starts the image calculation according to the specified parameters.
Cancel	Closes the dialog without executing the command.

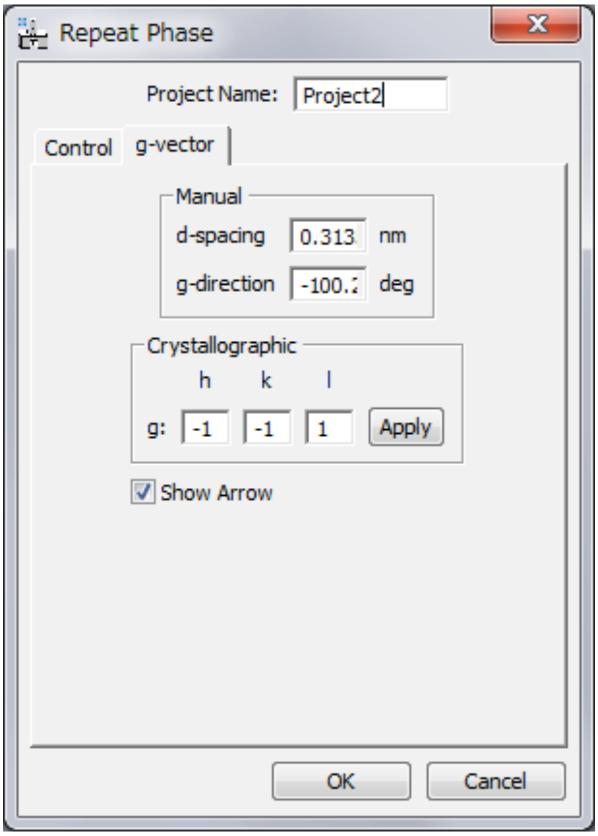
Control Tab



Component	Description
Display	Choice of results to be displayed.
Power Spectrum	Tick to display the power spectrum of the hologram.
Phase	Phase image is always displayed (hence grayed out).
Amplitude	Tick to display amplitude of holographic fringes (grayed out if not used previously).
Lattice-plane deformation	Tick to display corresponding lattice-plane

	deformation (grayed out if not used previously).
Options	Choice of image processing options. Not previously used options will be grayed out.
Define reference	Tick to define the reference in the same area as for the repeated project.
Distortion correction	Tick to apply the distortion correction as for the repeated project.
Reference hologram	Tick to use the reference hologram, which can be chosen from the scroll-down menu.
Fresnel Filter	Tick to apply the Fresnel Filter as for the repeated project. You can select the size of the filter.

g-vector Tab



Component	Description
Manual	Manual setup for the diffraction vector (g-vector) used to obtain the hologram.
d-spacing	Planar spacing in nm corresponding to g-vector.
g-direction	Angle of g-vector with respect to the image horizontal (anticlockwise positive).
Crystallographic	Crystallographic setup for the g-vector used to obtain the hologram. Please make sure the *correct* crystal settings have been defined (see Crystal tab).
g (h k l)	Miller indices of the diffraction vector.

Apply	Confirms the crystallographic definition. On click, d-spacing and g-direction calculated and displayed (and see Show Arrow). This button becomes active, only when the Crystal settings have been defined.
Show Arrow	Tick so that on Apply, an arrow is shown on original hologram image in the direction of the g-vector.

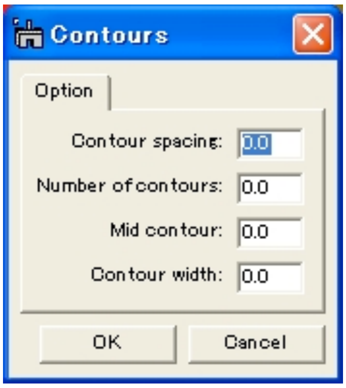
Phase Maths menu

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). If the phase images have been aligned, the new phase image will have a reference equal to the sum of the references of the two phase images. Otherwise, the new phase image will have a reference equal to the first phase image selected.
Subtract phase images	Subtracts two phase images (requested in a dialog box) and displays result in a third window (after phase renormalization). If the phase images have been aligned, the new phase image will have a reference equal to the difference of the references of the two phase images. Otherwise, the new phase image will have a reference equal to the first phase image selected.
Invert phase	Calculates the negative of the phase (and inverts the g-vector).

Phase Tools menu

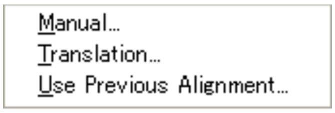
Option	Description
Sample by 2	Rebins the front-most phase image by two and multiplies the reference by two (thus preserving the reference values gx and gy in pixels^{-1} of the newly sampled image).
Contours	Superimposes contours on the front most image (see options).
Create moirés	Creates a moiré image 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 HoloDark so that they are recognized as phase images. Dialog boxes will appear asking for the value of references gx and gy in pixels^{-1}. Images which are imported together will be considered aligned. If the image has tags called Phase:gx and Phase:gy, these will be proposed as default.
Get unwrapped phase	Displays unwrapped phase image in new window. Note: there is no unique solution for phase unwrapping.

Contours dialog
(Option Tab)



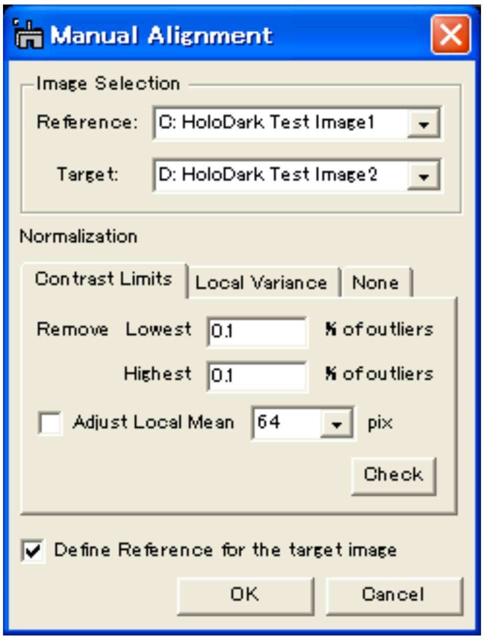
Component	Description
Contour spacing	Step in image values between each contour.
Number of contours	Total number of contours displayed.
Mid contour	Image value corresponding to mid contour.
Contour width	Contour line width in pixels.

Align Images menu



Option	Description
Manual	Starts Manual Alignment.
Translation	Starts translation-only automatic alignment. Any mouse clicks will be ignored when present.
Use Previous Alignment	Starts alignment using the previously determined alignment information. This alignment mode is useful, when the derived images give good alignment information.

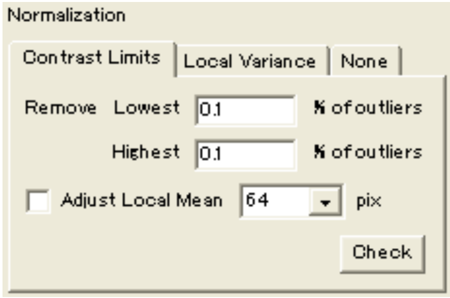
Manual Alignment Dialog



Component	Description
Image Selection	Choice of the two images to be used for alignment (usually Amplitude images, in which case the corresponding Phase images will be aligned accordingly).
Reference	Specify the Reference Image i.e. the one which will remain fixed.
Target	Specify the Target Image i.e. the one which will be shifted (magnified and rotated) to align with Reference image.
Normalization (see Scheme Tabs)	Manual alignment tool requires normalized images. Normalization scheme is selected from the Tabs.
Define Reference for	Tick to Define reference in the same area used for the

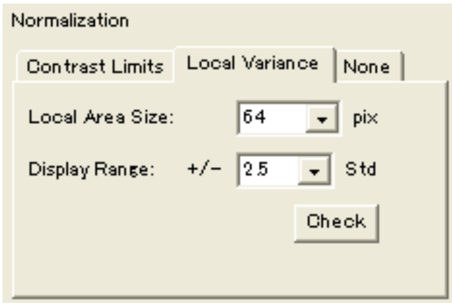
the target image	reference image.
OK	Closes the dialog and starts the procedure according to the specified parameters.
Cancel	Cancels the procedure.

Normalization
(Contrast Limits Tab)



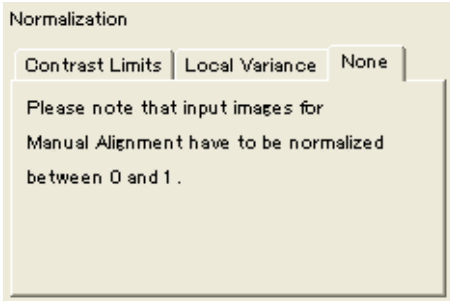
Component	Description
Remove outliers	Display limits (Lowest and Highest values) are defined by excluding the specified % of outliers (same as DM display limits).
Adjust Local Mean	Tick to adjust background using the local mean. The size of area used to calculate the local mean is specified in pixels.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

Normalization
(Local Variance Tab)

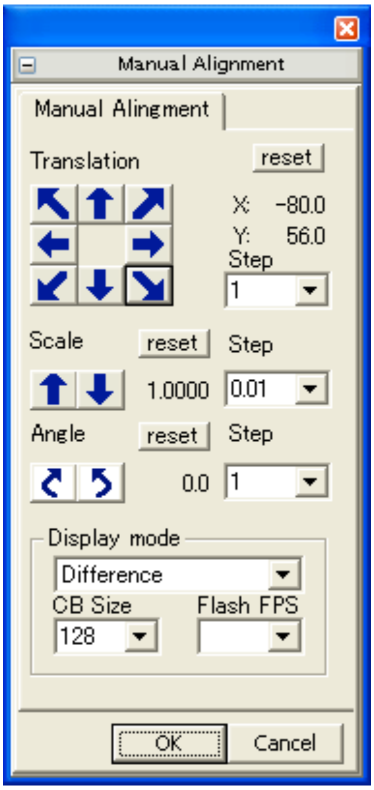


Component	Description
Local Area Size	Specifies a local area size in pixels.
Display Range	Specifies display range in terms of local standard deviation (std). Namely, the display range will be <local mean> +/- <display range>*<local std>.
Check	Click to check the effect of normalization.

Normalization
(None Tab)



Manual Alignment Tool



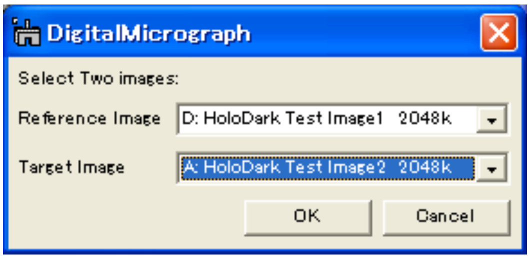
Component	**Description**
Translation	Translates the Target image with respect to the Reference image, in the direction of the arrow clicked upon. Keyboard arrow keys can also be used.
Reset	Returns the target image to its initial position.
Step	Step for one click in pixels.
Scale	Magnifies, or demagnifies, the Target image with respect to the Reference image.
Reset	Returns the Target image to its initial magnification.
Step	Step for one click in fractions of scale change.
Angle	Rotates the Target image, clockwise or anticlockwise, with respect to the Reference image.
Reset	Returns the Target image to initial orientation.
Step	Step for one click in degrees.
Display mode	Display mode may be selected from the pull-down list.

CB Size	Defines the checker board size (in pixels) for Checker Board display mode CB.
Flash FPS	Defines Image flash rate (in seconds) for Flash mode display. (Actual flash rate is hardware dependent.)

<u>Automatic Alignment</u>

● ***Translation***

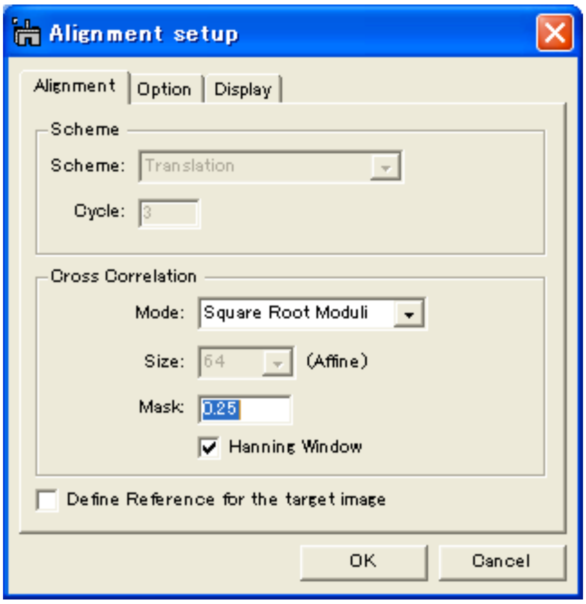
(Image Selection Dialog)



Option	Description
Reference Image	Specify the Reference Image i.e. the one which will remain fixed.
Target Image	Specify the Target Image i.e. the one which will be shifted (magnified and rotated) to align with Reference image.

<u>Translation Alignment</u>

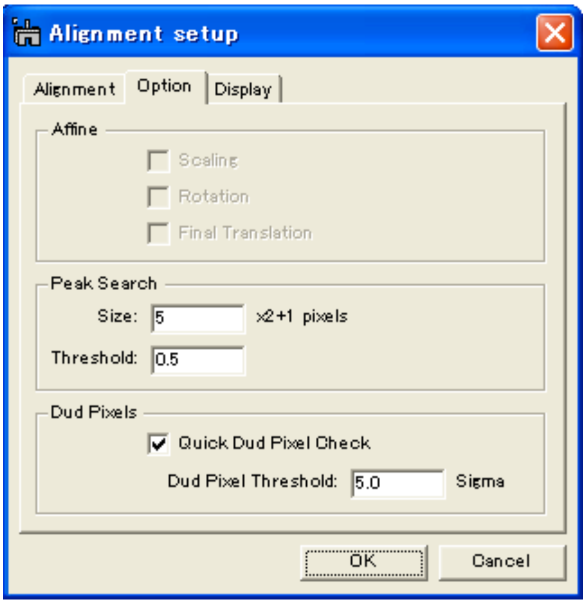
(Alignment Tab)



Option	Description
Scheme	
Scheme	(Translation)
Cross Correlation	
Mode	Cross-correlation mode will be selected from: *<u>Conventional</u>*: cross-correlation with normal amplitudes. *<u>Square Root Modulus</u>*: cross-correlation with square

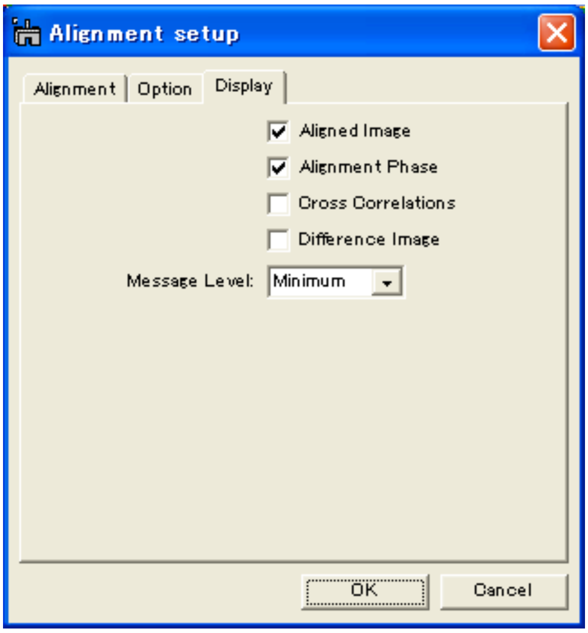
	root amplitudes. *Phase Only*: cross-correlation with unit amplitudes (only phase will be retained). *None*: No alignment.
Size	(Always use the whole image)
Mask	Specifies a radius of Low-pass filter in Fourier space (relative to the Nyquest frequency) to reduce high-frequency noise.
Hanning Window	When checked, a Hanning Window will be applied for Fourier transforms used for cross-correlation calculations.
Define Reference for the target image	Tick to Define reference in the same area used for the reference image.

Translation Alignment
(Option Tab)



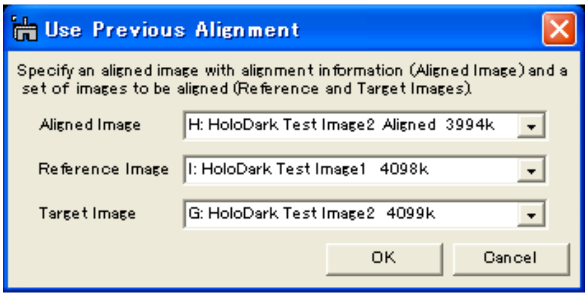
Option	**Description**
Peak Search	
Size	Radius of the cross-correlation peak search area.
Threshold	Intensity below this level will be ignored when estimating a peak center.
Dud Pixels	
Quick Dud Pixel Check	If checked, abnormal pixels will be checked based on the standard deviation of the whole image.
Dud Pixel Threshold	Specifies the threshold standard deviation for a quick dud pixel check.

Translation Alignment
(Display Tab)



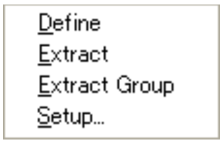
Option	Description
Aligned Image	Tick to display Reference and Target images after alignment.
Alignment Phase	Tick to display corresponding phase images after alignment.
Cross Correlations	Tick to display cross-correlation patterns.
Difference Image	Tick to display a difference between images used for alignment. This is useful to check an alignment quality.
Message Level	Controls the amount of output message to the Results Window. (None/Normal/Detail)

Automatic Alignment
●Use Previous Alignment
(Image Selection Dialog)



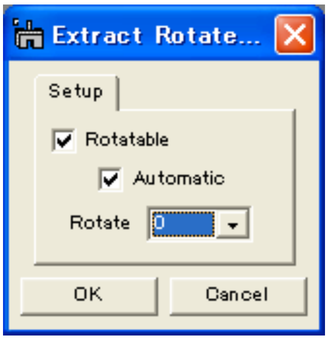
Option	Description
Aligned Image	Specify a previously aligned image.
Reference Image	Specify the Reference Image i.e. the one which will remain fixed.
Target Image	Specify the Target Image i.e. the one which will be shifted (magnified and rotated) to align with Reference image.

Extract Rotated Region menu



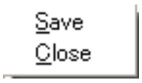
Option	Description
Define	Before running the command, an area needs to be selected by the DM rectangular ROI tool. The rectangular ROI can be made rotatable (see Setup).
Extract	Extracts the region within the ROI. The long edge direction will be rotated to horizontal. The final display can be further rotated by 90/180/270 degrees (see Setup).
Extract Group	Extracts the same area from a group of images (e.g. strain maps).
Setup…	Opens Setup Dialog.

Setup Dialog



Option	Description
Rotatable	Tick to make the rectangular ROI rotatable. Edge length will be adjusted by grabbing the yellow edges, and the rotation angle will be adjusted by the yellow cross (+). (You can change the both edge lengths by dragging the yellow cross when holding down the SHIFT key.).
Automatic	Tick to align initially the reference ROI parallel to the hologram fringes.
Rotate	The selected region will be displayed with further rotation by 90/180/270 degrees.

Image Group menu



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

Reference Image menu

Component	Description
Save As	Saves the original 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.