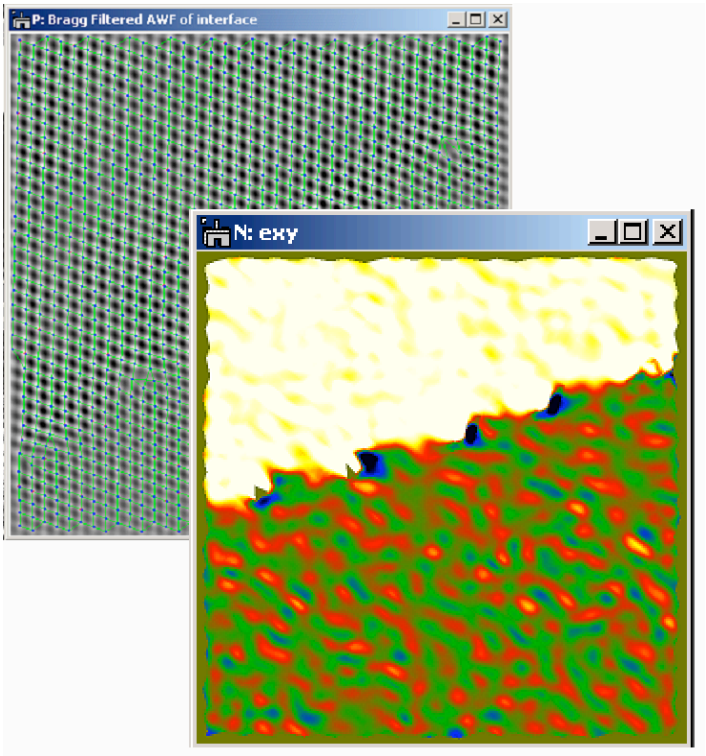
2008/OCT

PPA for DigitalMicrograph

Peak Pairs Analysis

High-Resolution Peak Measurement
and Strain Mapping Analysis



PPA User Manual v1.0

HREM Research Inc

Contact Information

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Introduction to Peak Pairs Analysis (PPA)

PPA stands for Peak Pairs Analysis, the DigitalMicrograph plug-in for High-Resolution Peak Measurement and Strain Mapping Analysis.

All results obtained by PPA are fully compatible with the other functions present in DM. For example, strain maps can be analysed and/or manipulated with functions such as histograms, statistics (mean, standard deviation, min, max etc.), or using the corresponding buttons, such as the Profile utility.

The main reference for the algorithm is:

> *The Peak Pairs algorithm for strain mapping from HRTEM images*
> Pedro L. Galindo, Sławomir Kret, Ana M. Sanchez, Jean-Yves Laval, Andrés Yáñez, Joaquín Pizarro, Elisa Guerrero, Teresa Ben and Sergio I. Molina
> Ultramicroscopy 107 (2007) 1186–1193
> *doi: 10.1016/j.ultramic.2007.01.019*

This manual will help you to use of the PPA package with some worked examples.

Software requirements

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

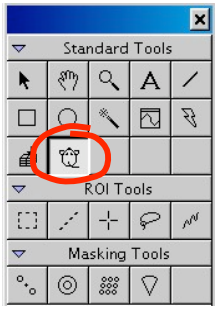
- DigitalMicrograph (GATAN™)
- USB Key Driver
- Mouse Tools

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 PPA, or you can find it on our web site.

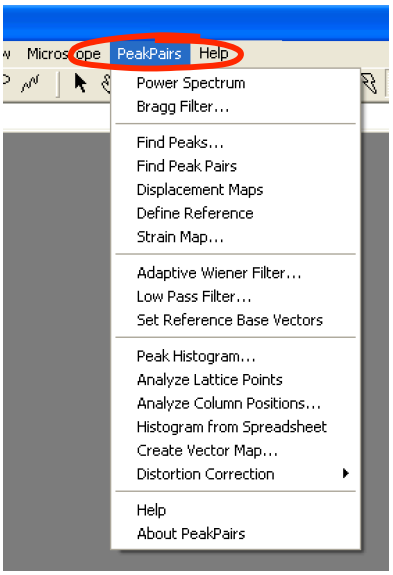
Installing Mouse Tools



All the files relating Mouse tool plug-in can be installed by drag-and-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 PPA



PeakPairs.gtk and PeakPairs.dll can be installed by drag-and-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, PeakPairs menu commands will appear under "PeakPairs" menu.

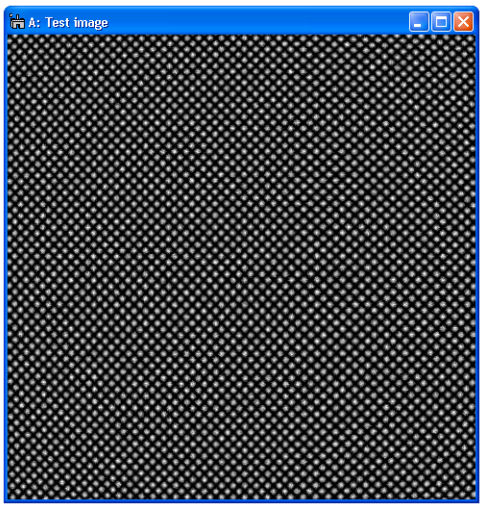
MKL Library

One file for the Intel MKL library should be copied to the same level of DigitalMicrograph. This file comes with PPA plug-in.

Getting Started

Image preprocessing and Basis Vector Selection

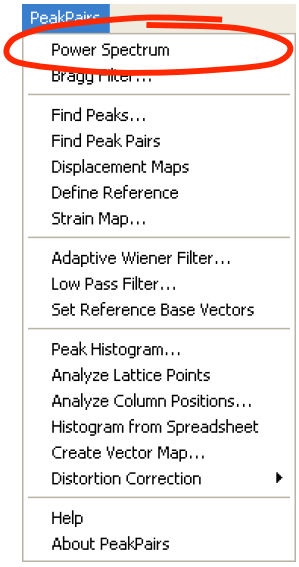
Open the file "Test image.dm3" using the DM command **File…Open**:

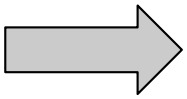


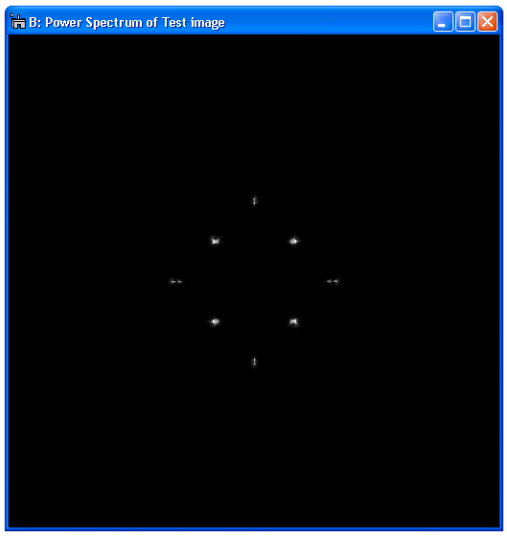
Hint: this image has been generated artificially to show PPA functionality.

It consists on a dot pattern where different strains are present, but not visible at the naked eye.

All the commands related to PPA are located in the menu **Peak Pairs**. The first command to be applied to a new image is to calculate the *Power Spectrum* of the image:

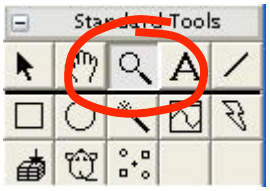


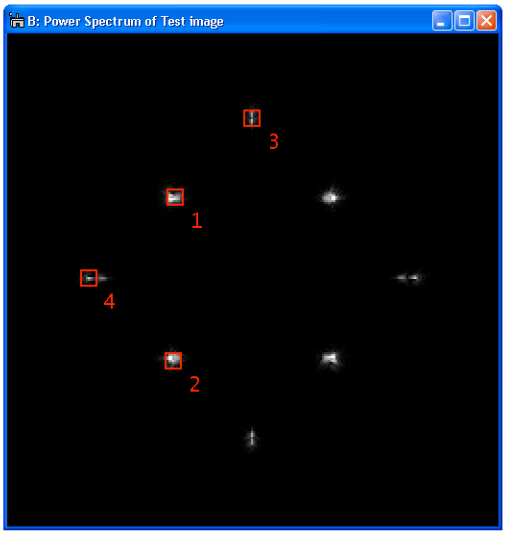




Now, using the **mouse tool,** click on desired spots. The usual choice is to select the brightest spots in the spectrum, but those corresponding to higher harmonics can also be selected:

The user doesn't need to hit the spot exactly, because PPA looks for the local maxima near the selected point. Anyway, you can zoom in the spectrum before hitting peaks using the DM **zoom** tool:





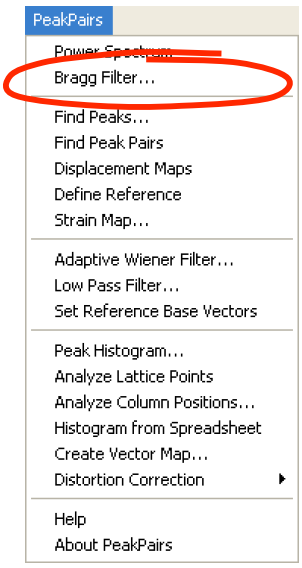
Hint: if you wish to delete any spot, just click on the mouse mark again with the SHIFT key down.

Hint: Symmetry in the selection for each spot is assumed.

IMPORTANT: First and second chosen spots (numbered as 1 and 2) will define the lattice basis vectors. These spots should be apart from the vertical or horizontal of the central spot, in order to obtain maximum resolution.

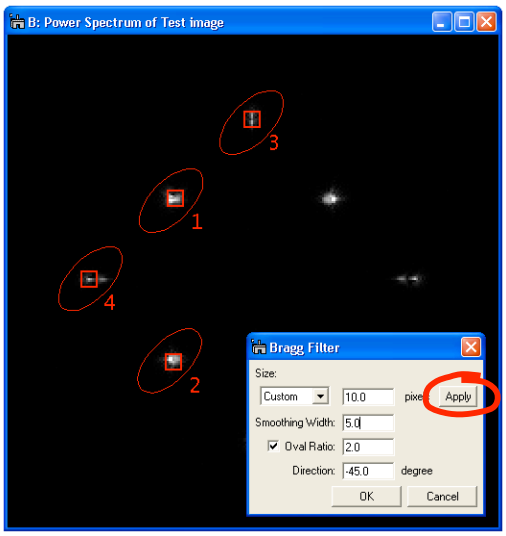
Don't be surprised if the central spot is not present in the power spectrum. It just indicates that the mean intensity of the image is zero.

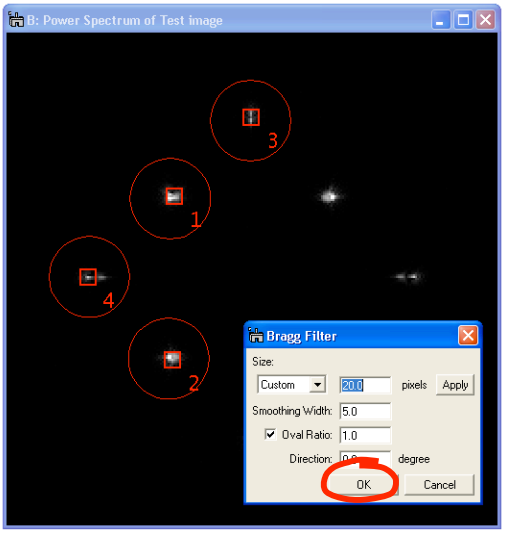
We are now ready to apply a Bragg Filter. This process creates an image where the contrast resulting from the ordered regions is clearly distinguishable from the background intensity.



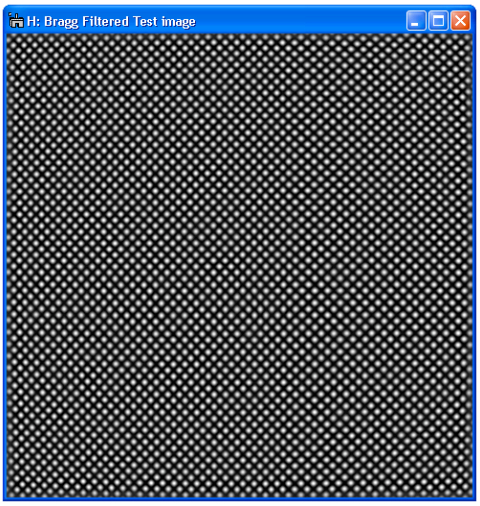
The shape and size of the Bragg filter must be adjusted such that no loss of information occurs. In this dialog box we can determine the size (in pixels), smoothing width(in pixels), oval ratio(height/width) and direction(in degrees) of mask spots.

By pressing the *Apply* button, the mask described by the chosen parameters may be previsualized, as it is shown in these two examples:



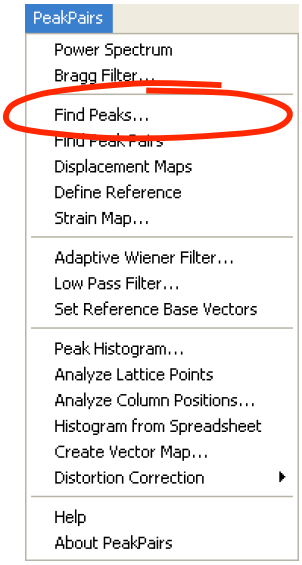


Let us select the second choice by pressing the OK button, and the Bragg filtered image will appear immediately.



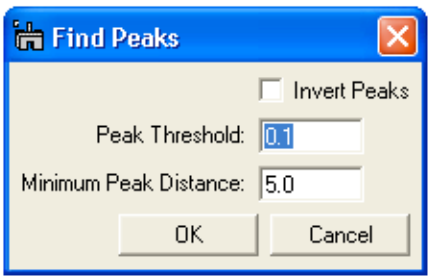
If Bragg filter parameters are properly chosen (big masks and a sufficient number of peaks), the resulting filtered image will preserve the location of maxima. The great advantage in using the filtered image is the reduction of present noise.

Peak Pairs Determination

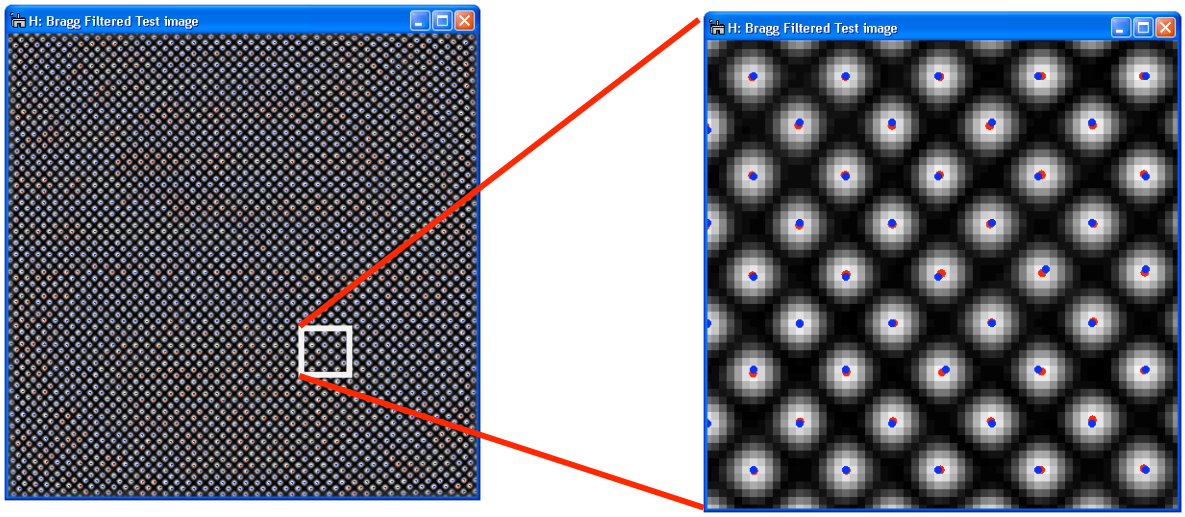


Once we have a Bragg filtered image, the next step is to locate peaks of intensity in the image by pressing the *Find Peaks* option.

The following dialog box appears:



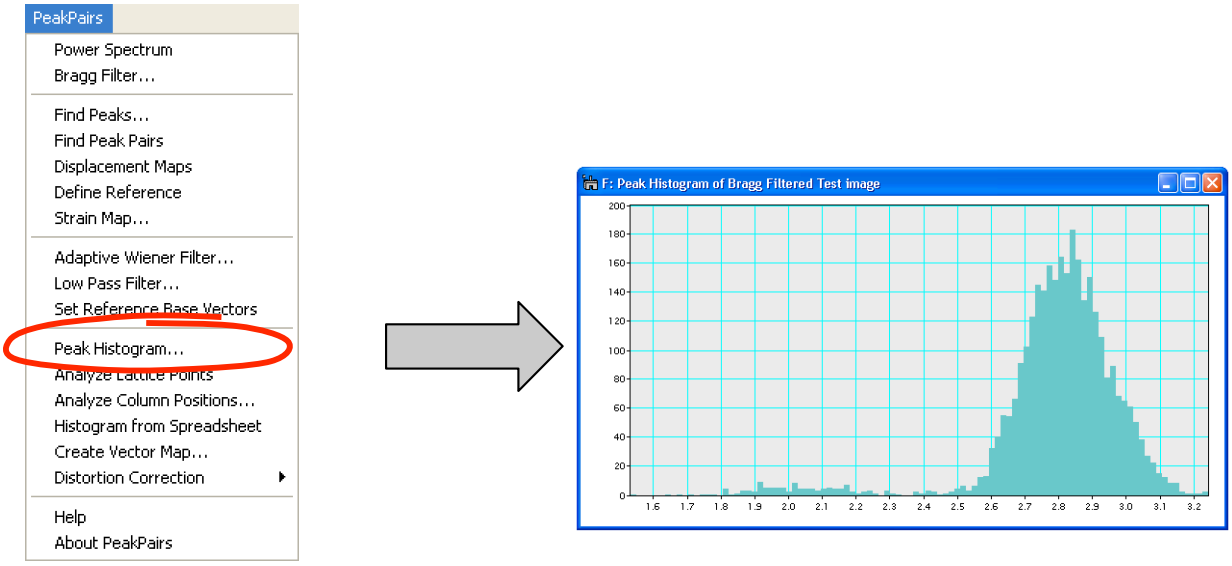
Note: Let's ignore by now the parameters in the checkbox. They will be discussed later.



By pressing OK, we get a first set of peaks shown as coloured spots over the filtered image. Blue dots represent local maxima (8-neighbourhood) on a pixel basis. Red dots represent refined maxima at subpixel-resolution. Sub-pixel resolution is achieved by fitting a 2D quadratic function and calculating analytically the maxima, as described in [1].

Sometimes, extra peaks are obtained in this automatic Peak Finding process, especially at the borders of the image.

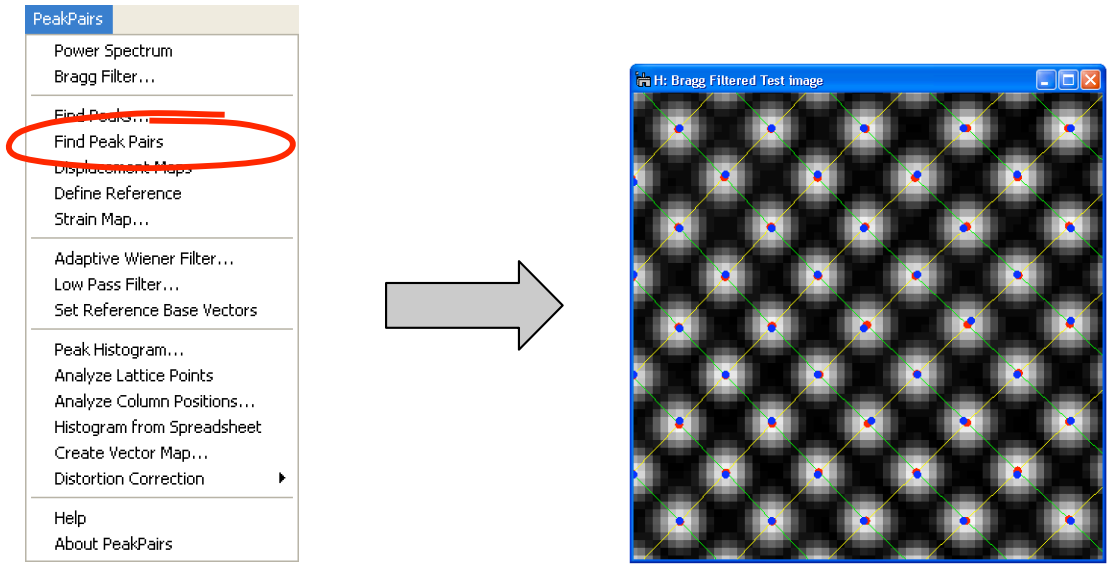
Peak Threshold indicates the minimum intensity of a point to be considered as a valid peak. Peaks having intensities below this threshold will be discarded. To determine a precise value of Peak Threshold, a Peak Histogram may be very useful. This can be obtained using the corresponding option in the Peak Pairs menu.



By looking at the histogram, a reasonable threshold could be the value 2.5. Repeating the Find Peaks command and choosing Peak Threshold=2.5, all peaks in the border of the image will be discarded and won't be considered in any further calculations.

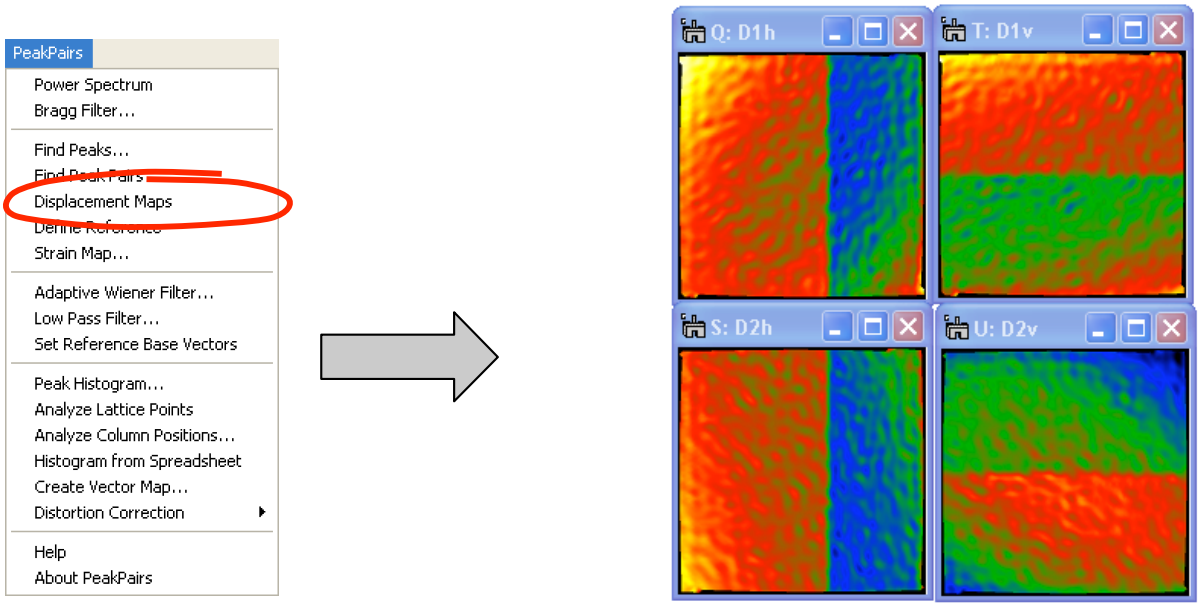
If we want to restrict the distance between peaks, it is possible to define the Minimum Peak Distance in the same dialog box.

The next step is the calculation of Peak Pairs. This process will find pairs of peaks along two basis vectors automatically chosen from the user selected Bragg spots (see Additional functions for selecting the reference basis vectors manually).



Once all Peak Pairs have been determined, we can proceed to the calculation of displacement maps using the command *Displacement Maps*. This generates horizontal and vertical displacements along the two defined directions (D1h, D1v, D2h and D2v).

Displacement and Strain Maps calculation



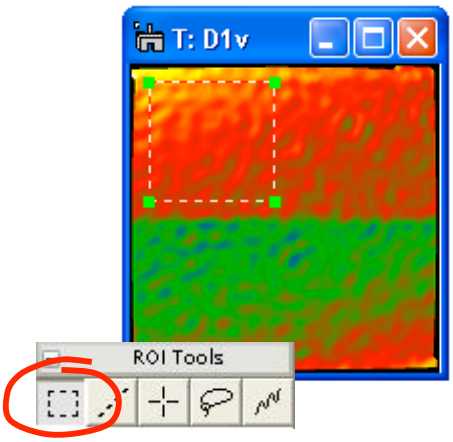
Technical note: PPA uses an automatic selection of contrast and the temperature colour scale for displaying image values.

If you prefer a grey scale or a different contrast limit, press the right button on the image, and modify ImageDisplay options properly.

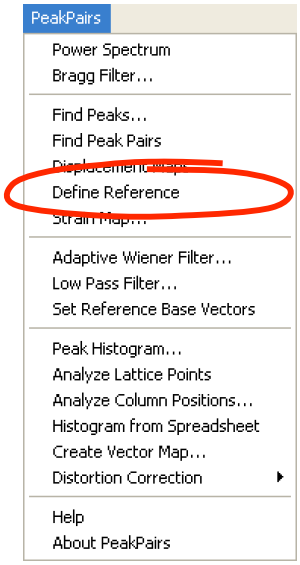
Changing this options will not change the actual values, only its appearance.

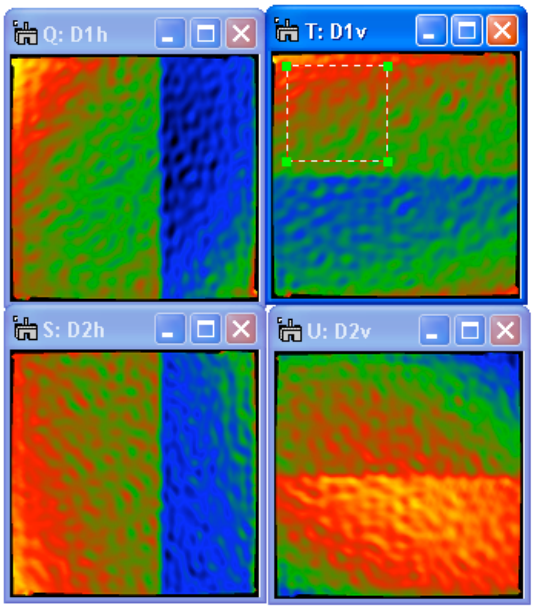
A **very important step** is to define the reference area, that is to say, the area which is considered to correspond to the reference lattice.

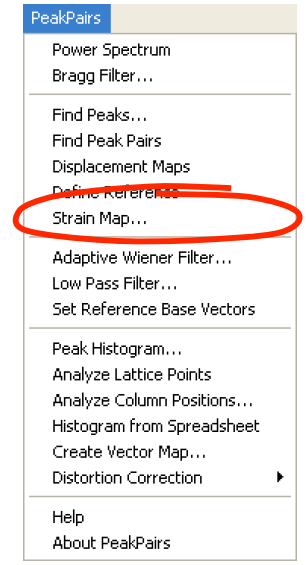
All displacements and strain values will be referred to this area. Use the DM **ROI tool** (region of interest tool) to select an area on any Displacement image (D1h, D1v, D2h or D2v):

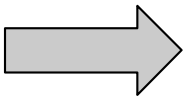


Once the reference area has been chosen, the user should select the Define Reference option. This will change the displacement values, so as to obtain a uniform displacement in the chosen area.

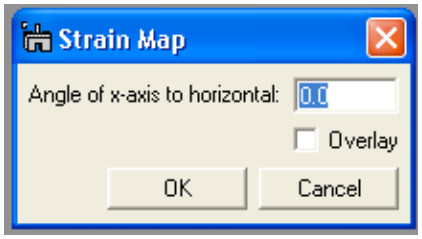




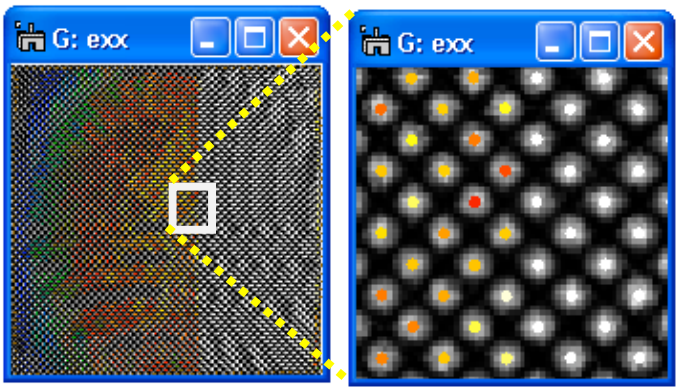




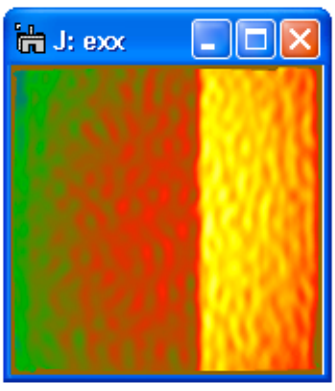
The final step is the determination of strain maps (e_{xx},e_{yy},e_{xy} and e_{yx}) at the desired angle. If angle is set equal to 0, horizontal and vertical directions are assumed to be x and y coordinate axis respectively.



There are two options for strain representation:



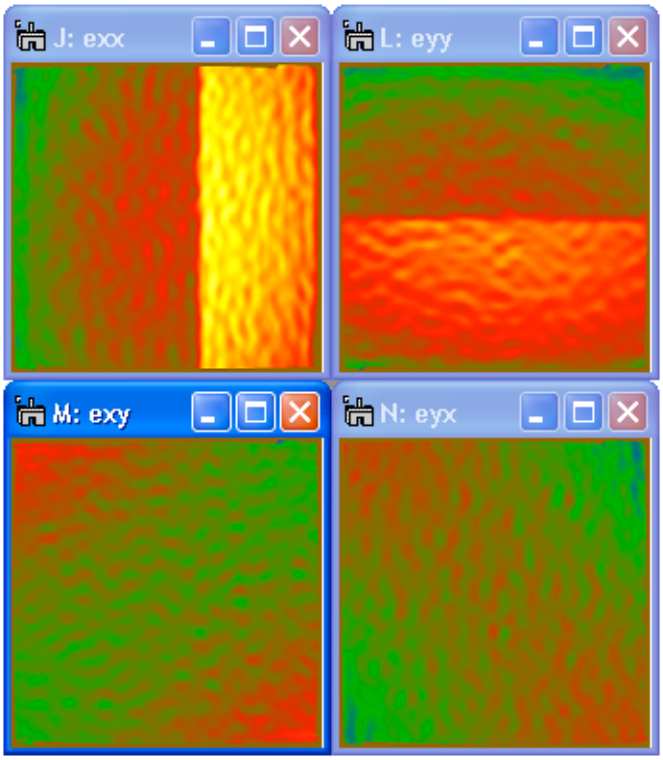
Overlay: the strain is shown at each atomic column, and displayed as coloured dots over the original image



No overlay: continuous strain maps are shown.

Once the representation is chosen, a set of 4 images corresponding to (e_{xx},e_{yy},e_{xy} and e_{yx}) are obtained

Choosing the *x-axis* parallel to the picture horizontal axis (i.e. angle zero) and leaving overlay unmarked, the following image group will be obtained:



Hint: you can modify the color range by pressing the right button of the mouse on the image, and modifying ImageDisplay options properly.

Default colour range is ±5%

The results of the PPA package is the complete strain tensor defined as follows:

Strain values

$$e_{xx} = \frac{\partial u_x}{\partial x},\ e_{yy} = \frac{\partial u_y}{\partial y},\ e_{xy} = \frac{\partial u_x}{\partial y},\ e_{yx} = \frac{\partial u_y}{\partial x}$$

Strain tensor:

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

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):

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

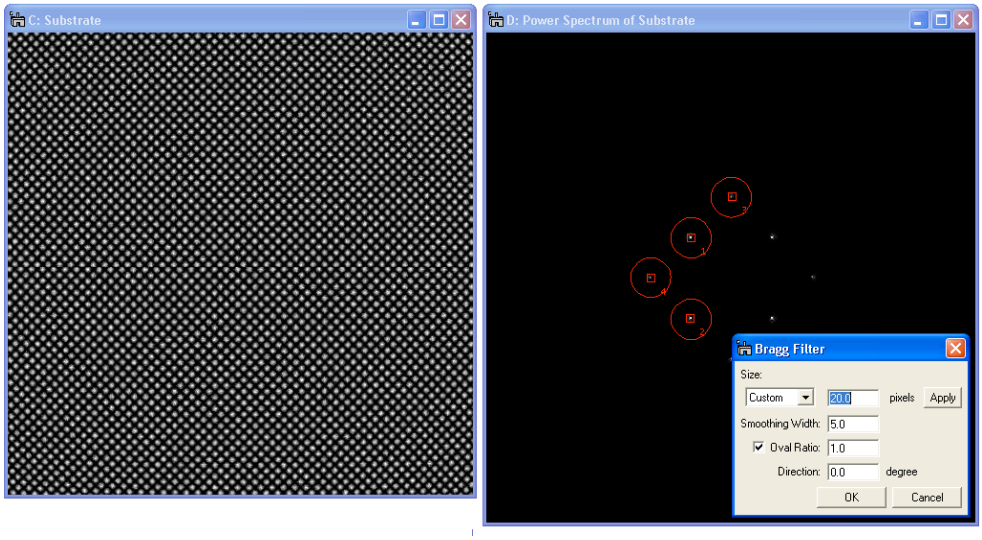
As we clearly see in the resulting images, the displacement and strain maps appear to be the composition of two different sources of deformation. The reason is that distortions due to the projector lens have been made quite visible in the example.

In the next section, we will show how to remove this distortion using an image of a perfect crystal taken in the same conditions.

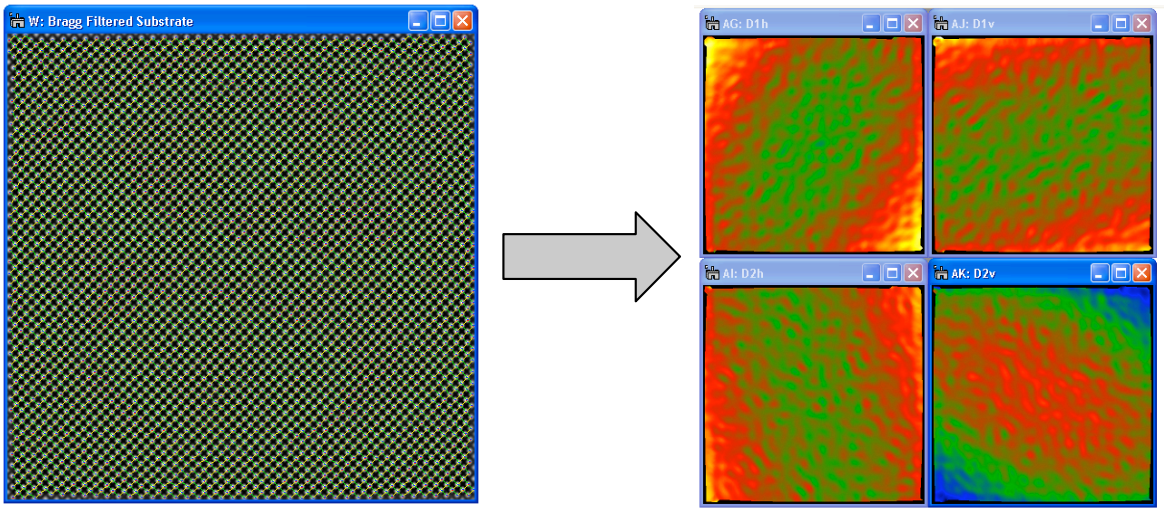
Geometric distortion correction

All optical systems distort the images they form. CCD cameras and scanners (for digitising negatives for example) introduce additional distortions. If these geometric distortions are fixed (what is usual for a given system), it is possible to eliminate them. This is valid not only for projector lens distortions but also for any other systematic distortions present in the image.

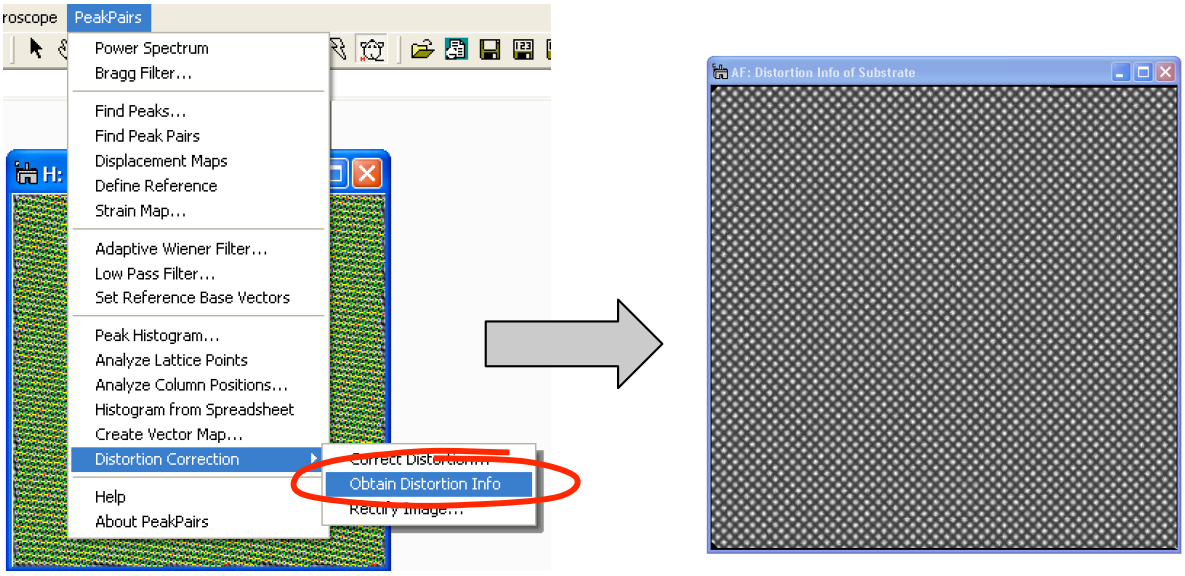
In order to correct the distortions, an image of a perfect crystal is needed. Open the image "Substrate.dm3", which corresponds to a perfect crystal image, calculate the *Power Spectrum,* and Bragg-filter the image in the usual way, by selecting relevant spots in the Power Spectrum and using a custom mask at each spot.



Then calculate the Peak Pairs using the usual commands (*Find Peaks* followed by *Find Peak Pairs*). If we analyze the displacements, we can observe that the image of a perfect crystal is shown distorted.

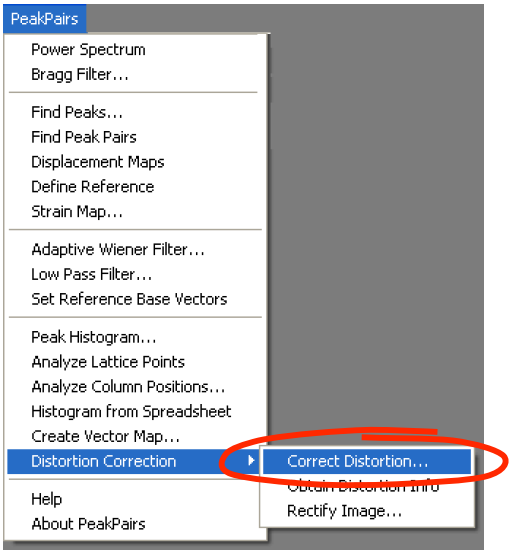


The distortion information that allows rectifying the perfect crystal image can be used to correct distortions in any other image with the same distortion. In order to do so, we have to the extract distortion information just selecting the Bragg image of the original crystal, and applying the command *Obtain Distortion Info.*

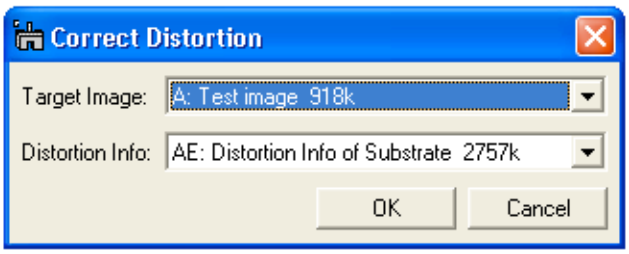


This Distortion info image can be saved to disk and used in further analysis having the same distortion.

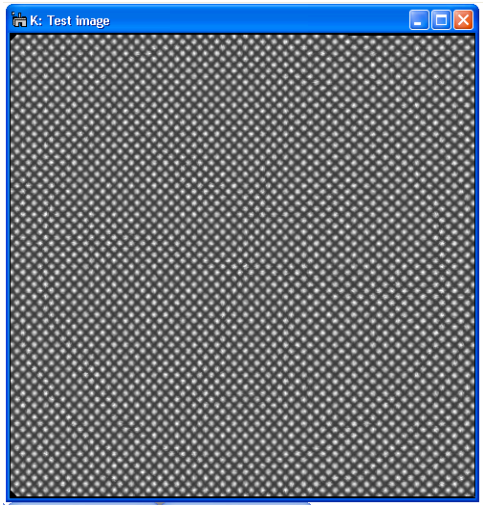
In order to rectify the original image with the distortion information obtained from the perfect crystal image, just apply the Correct Distortion on the Target Image using the Distortion information obtained from the reference (Perfect Crystal), as follows:



1. Open the Correct Distortion dialog
2. Select the Target Image (Test Image)
3. Select the Distortion Info (Distortion Info of Substrate)

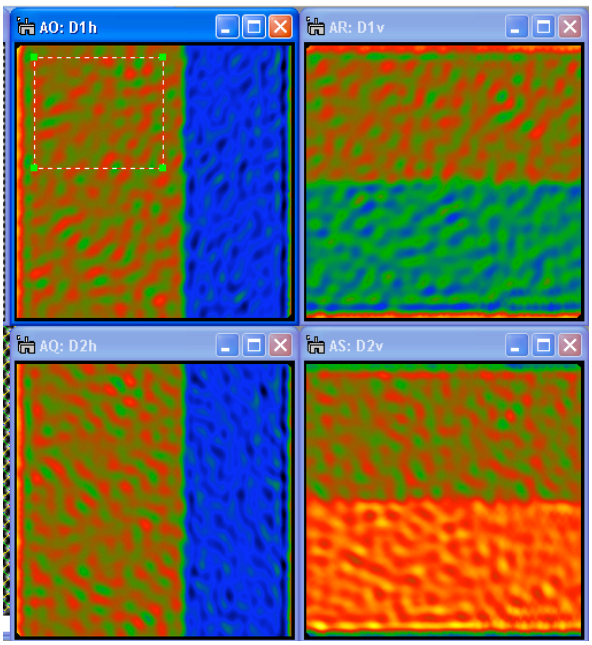


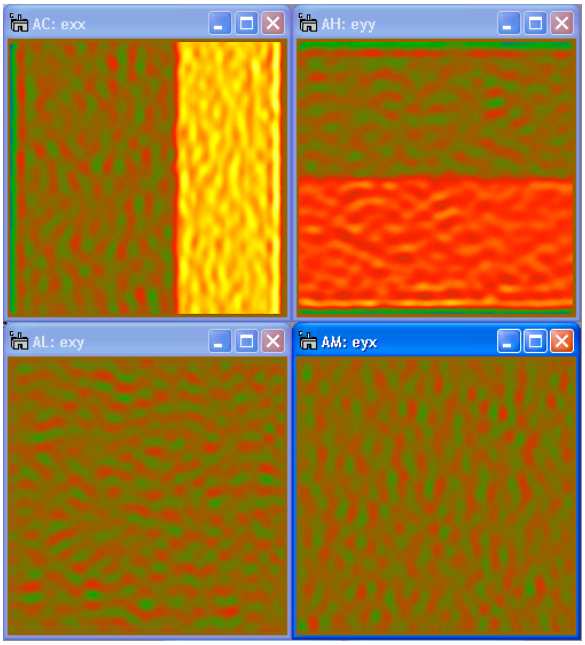
This will produce a corrected image, where all distortions due to the microscope have been eliminated.



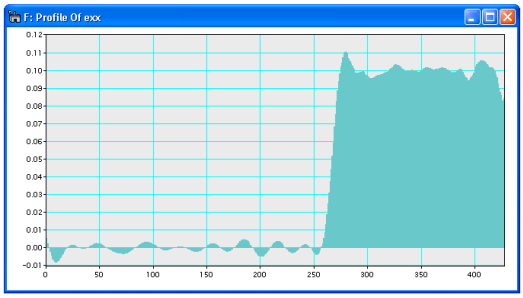
We can now proceed to analyze this image in the usual way to get the final results:

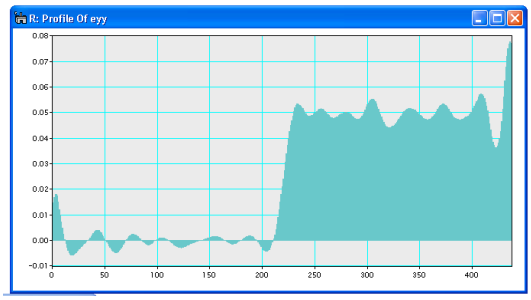
1. Power Spectrum
2. Bragg Filtering
3. Find Peaks
4. Find Peak Pairs
5. Displacement Maps
6. Define reference
7. Strain maps





If we plot a horizontal profile across exx and a vertical one across eyy, we get the expected results (exx=0.1 and eyy=0.05).



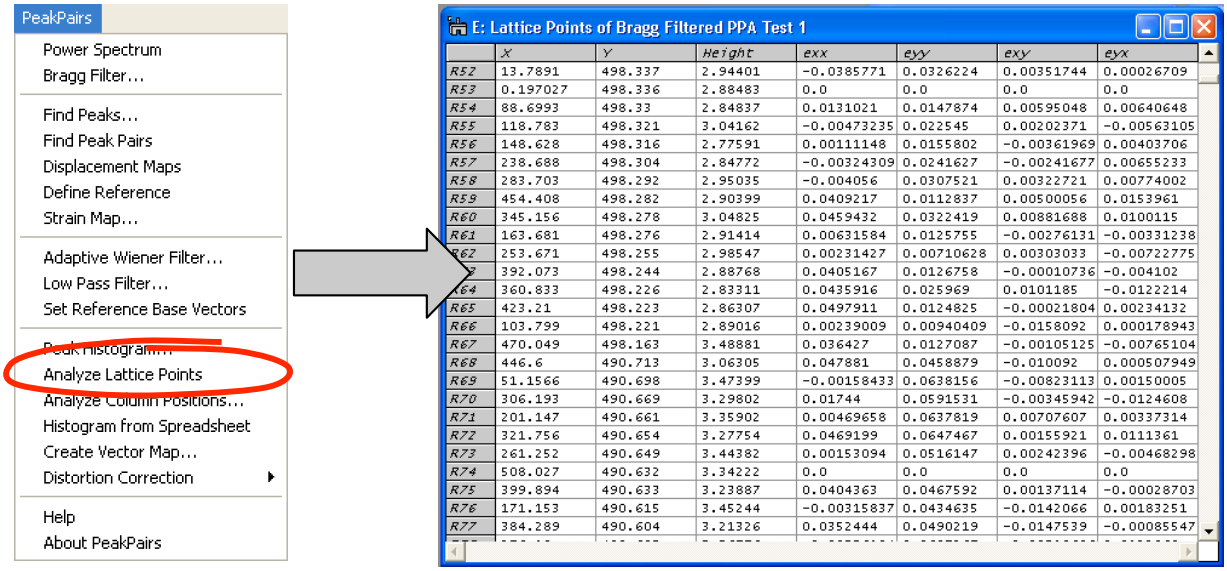


Additional functions

Lattice Analysis

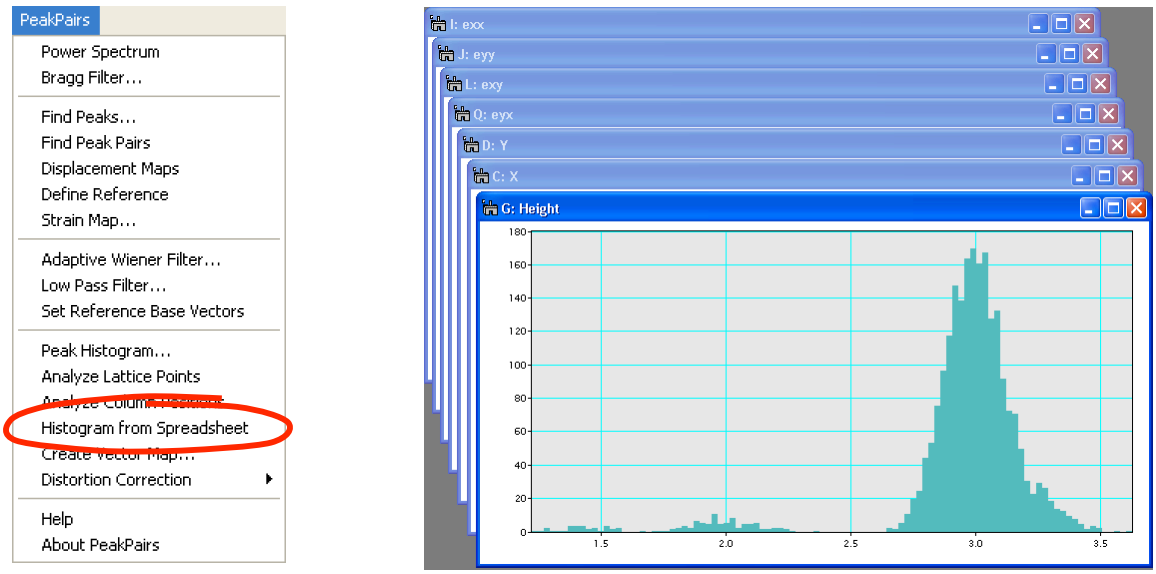
Selecting the Bragg filtered image after Peak Pairs, displacements maps and strains calculation, and using the Analyze lattice points command will generate a spreadsheet including the following columns (one row for each each lattice peak):

- Peak position at subpixel resolution (x,y coordinates)
- Peak intensity (gray level)
- Atomic column strain tensor (exx,eyy,exy and eyx).



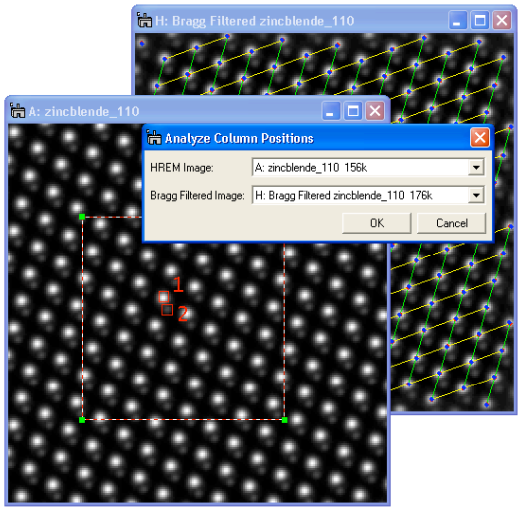
	X	Y	Height	exx	eyy	exy	eyx
R52	13.7891	498.337	2.94401	-0.0385771	0.0326224	0.00351744	0.00026709
R53	0.197027	498.336	2.88483	0.0	0.0	0.0	0.0
R54	88.6993	498.33	2.84837	0.0131021	0.0147874	0.00595048	0.00640648
R55	118.783	498.321	3.04162	-0.00473235	0.022545	0.00202371	-0.00563105
R56	148.628	498.316	2.77591	0.00111148	0.0155802	-0.00361969	0.00403706
R57	238.688	498.304	2.84772	-0.00324309	0.0241627	-0.00241677	0.00655233
R58	283.703	498.292	2.95035	-0.004056	0.0307521	0.00322721	0.00774002
R59	454.408	498.282	2.90399	0.0409217	0.0112837	0.00500056	0.0153961
R60	345.156	498.278	3.04825	0.0459432	0.0322419	0.00881688	0.0100115
R61	163.681	498.276	2.91414	0.00631584	0.0125755	-0.00276131	-0.00331238
R62	253.671	498.255	2.98547	0.00231427	0.00710628	0.00303033	-0.00722775
R63	392.073	498.244	2.88768	0.0405167	0.0126758	-0.00010736	-0.004102
R64	360.833	498.226	2.83311	0.0435916	0.025969	0.0101185	-0.0122214
R65	423.21	498.223	2.86307	0.0497911	0.0124825	-0.00021804	0.00234132
R66	103.799	498.221	2.89016	0.00239009	0.00940409	-0.0158092	0.000178943
R67	470.049	498.163	3.48881	0.036427	0.0127087	-0.00105125	-0.00765104
R68	446.6	490.713	3.06305	0.047881	0.0458879	-0.010092	0.000507949
R69	51.1566	490.698	3.47399	-0.00158433	0.0638156	-0.00823113	0.00150005
R70	306.193	490.669	3.29802	0.01744	0.0591531	-0.00345942	-0.0124608
R71	201.147	490.661	3.35902	0.00469658	0.0637819	0.00707607	0.00337314
R72	321.756	490.654	3.27754	0.0469199	0.0647467	0.00155921	0.0111361
R73	261.252	490.649	3.44382	0.00153094	0.0516147	0.00242396	-0.00468298
R74	508.027	490.632	3.34222	0.0	0.0	0.0	0.0
R75	399.894	490.633	3.23887	0.0404363	0.0467592	0.00137114	-0.00028703
R76	171.153	490.615	3.45244	-0.00315837	0.0434635	-0.0142066	0.00183251
R77	384.289	490.604	3.21326	0.0352444	0.0490219	-0.0147539	-0.00085547

It is also possible to get a histogram from the Spreadsheet by using the *Histogram from Spreadsheet* command, thus obtaining a different histogram for each column in the spreadsheet.



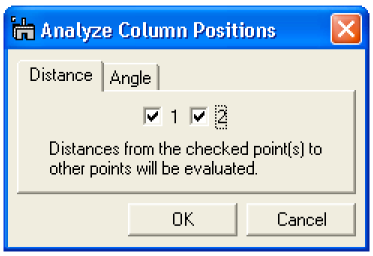
Analyze column positions

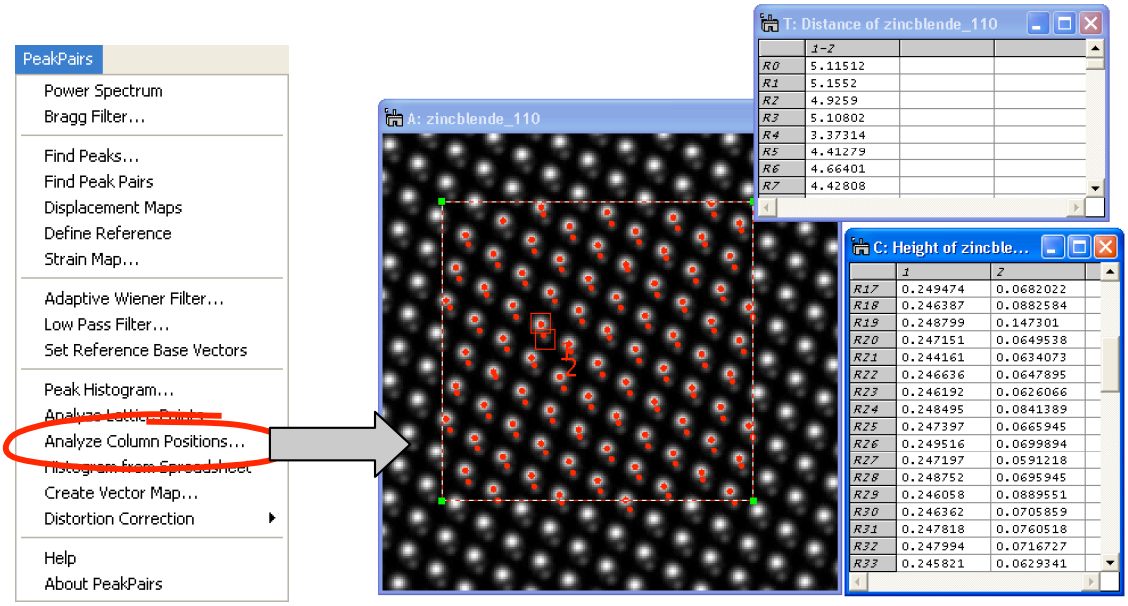
Once Peak Pairs have been located, it is possible to analyze column positions with respect to its relative position within the grid. This is very useful when more than one atomic column is present for each lattice point. For example, in the case of zincblende materials in the [110] direction, we can evaluate peak intensities at cation and/or anion column positions. In order to do so, go through the following steps:



- Calculate Peak Pairs in the usual way
- Use the rectangleROI tool to choose the area of interest in the original image
- Choose the point(s) of interest inside the image (i.e. any local maxima of intensity)
- Apply the *Analyze Column Positions* command
- Select the image and Bragg Filtered images in the corresponding dialog

Then, the user will have the option to decide between calculating the distances from the checked point to other points, or the angles subtended by two adjacent points. The results will be shown in the image, and the peak intensity at each point will be stored in a datasheet.

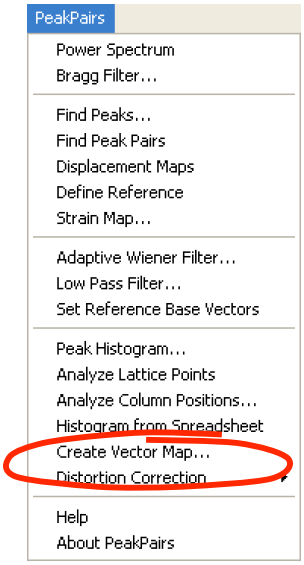


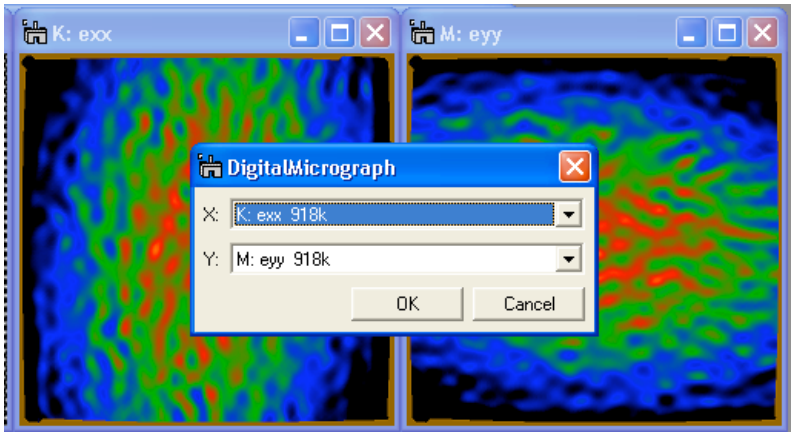


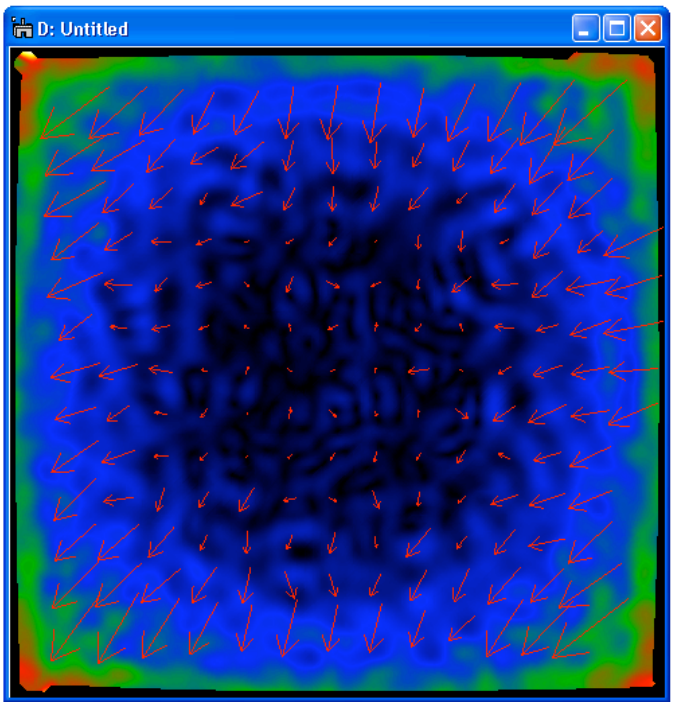
The number of columns in the datasheet will be equal to the number of points of interest chosen by the user.

Create Vector maps

It is possible to create vector maps from strain maps. To do so, just select the Create Vector Maps command after a complete strain analysis has been made. Then, select two strain maps in order to determine the associated vector map.



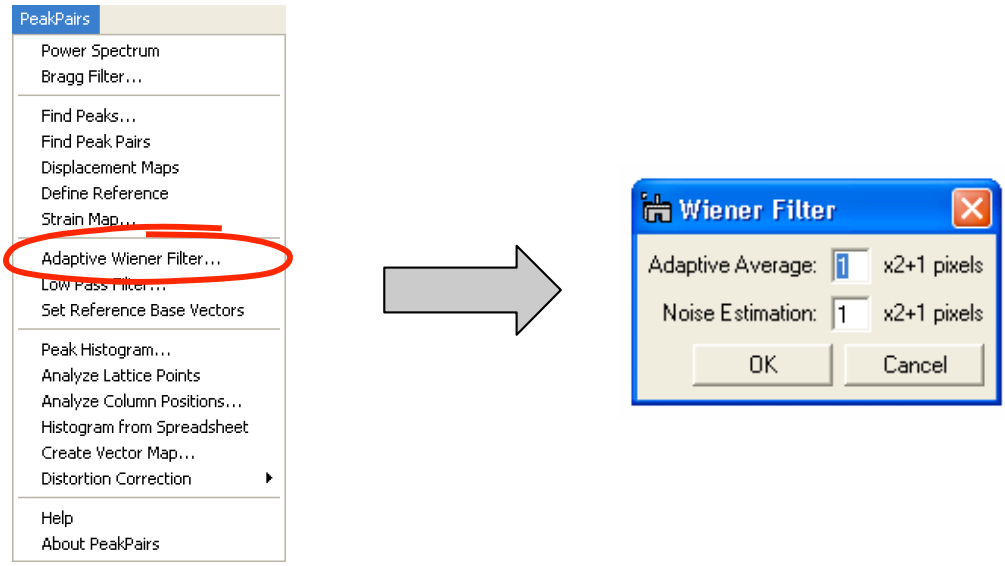




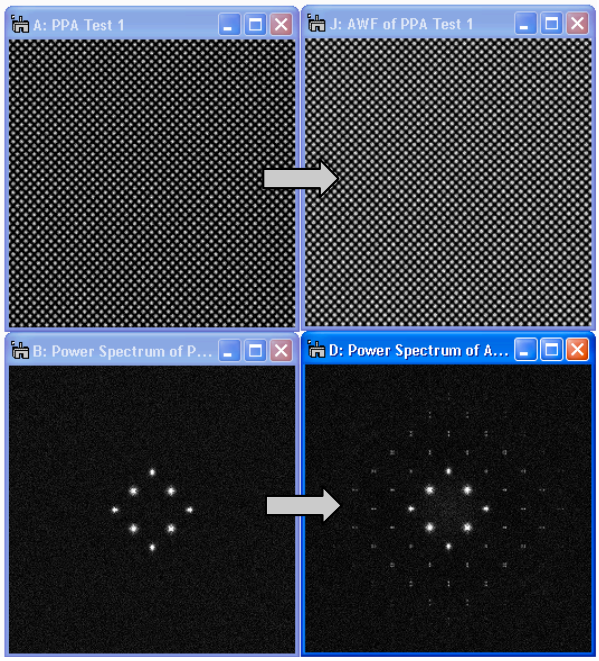
Adaptive Wiener Filtering

The Wiener filter is widely used for image restoration and calculates the optimal filter for the removal of noise from a signal which is corrupted by the measuring process itself. It assumes that if noise is present in the system, then it is considered to be additive white Gaussian noise.

After selecting the original image, and applying the Adaptive Wiener Filter in the menu, the user should decide the size of the windows used for calculating the Adaptive Average and the Noise Estimation, as follows:

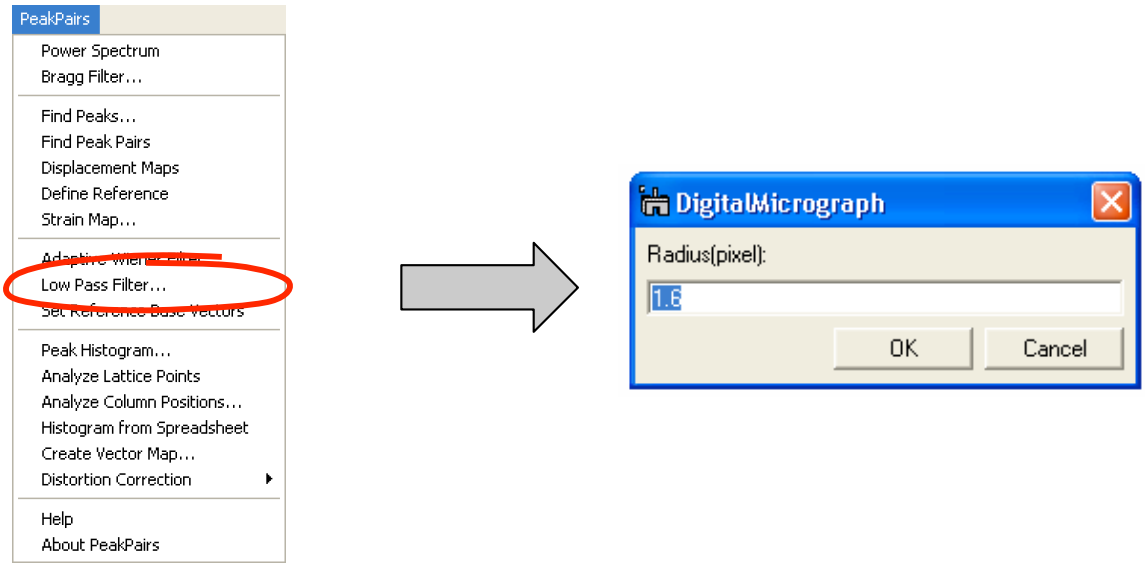


In a typical Peak Pairs session, if Wiener filtering is desired, it is usually the first operation to be applied to the original image. The result of the Wiener filtering operation on *PPA Test1* image and respective Power Spectra (Adaptive Average =3, Noise Estimation=3) is depicted below.

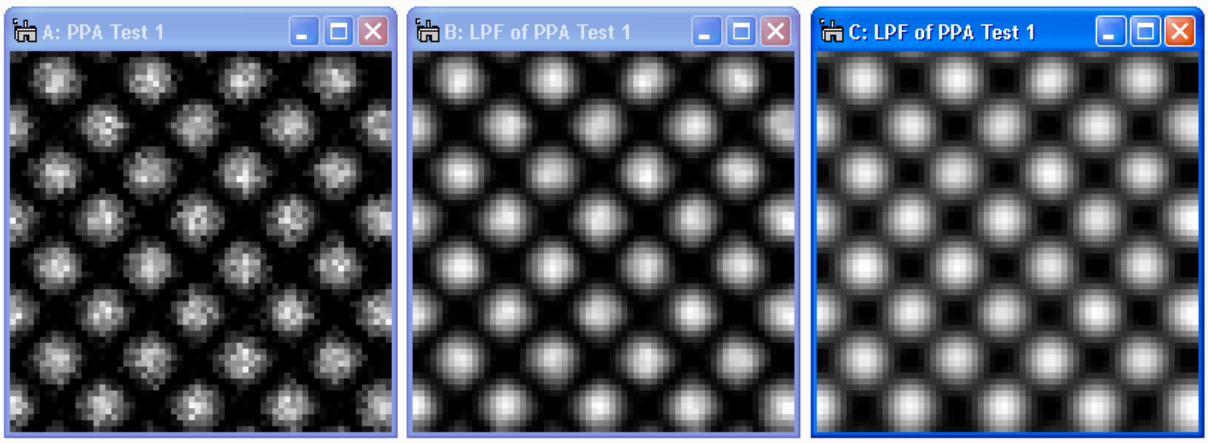


Low Pass Filtering

In order to generate a Low-Pass filtered image, we simply select the input image and use the *Low Pass Filter* command in the menu. The strength of the filter is defined by the radius of the mask in pixels (the highest the radius, the strongest the filter):



In the following figure, the resulting images after the application of a Low-Pass filter to the lower left part of *PPA Test1* image with different radius are shown:



Original image
(right-lower corner only)

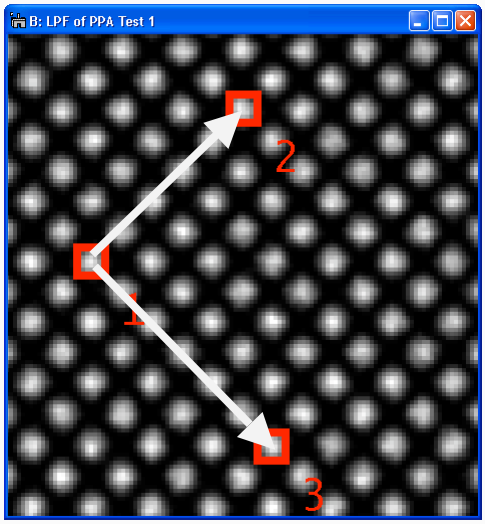
Low Pass Filtered
(radius=0.8 pixels)

Low Pass Filtered
(radius=1.6 pixels)

Setting the Reference Base Vectors manually

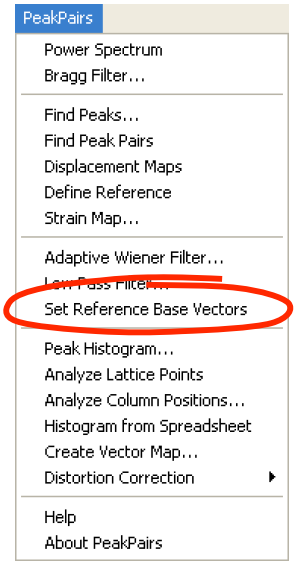
It is possible to manually set the reference base vectors. In order to do so, we need a filtered image, obtained using available options (Bragg or Low-Pass filtering).

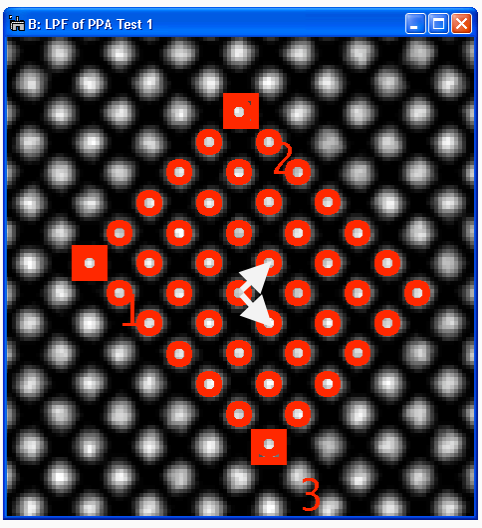
Once a filtered image has been selected, to manually define the Reference Base vectors, use the Mouse Tool to select 3 points in the order (origin of both vectors, terminal point of vector 1, terminal point of vector 2), so that the directions of the desired reference base vectors are described approximately by the directions of vectors $\vec{12}$ and $\vec{13}$.



Approximate directions
as described by the user

The precise magnitude and direction of both reference base vectors are calculated, when applying the *Set Reference Base Vectors* command, as the average of all the vectors included in the parallelogram described by these 3 points having their extremes at intensity maxima peaks and the same approximate directions.



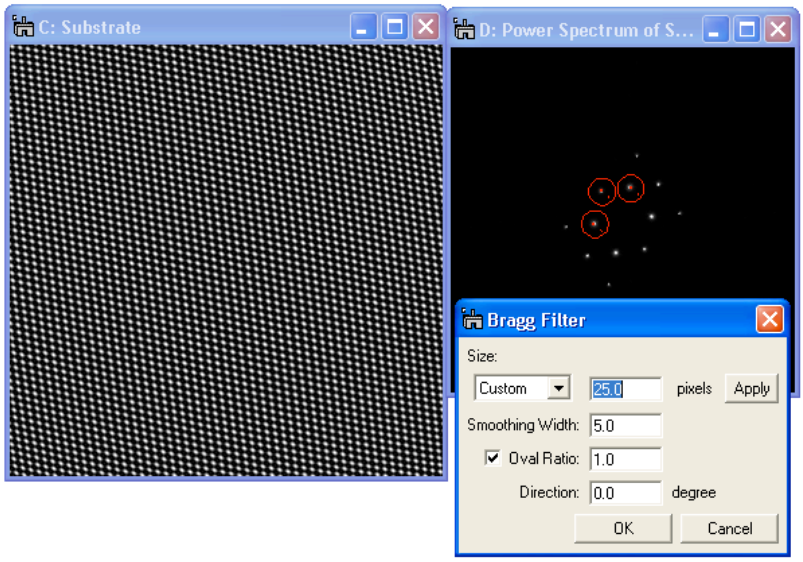


Reference Base Vectors
(average of all vectors in this area)

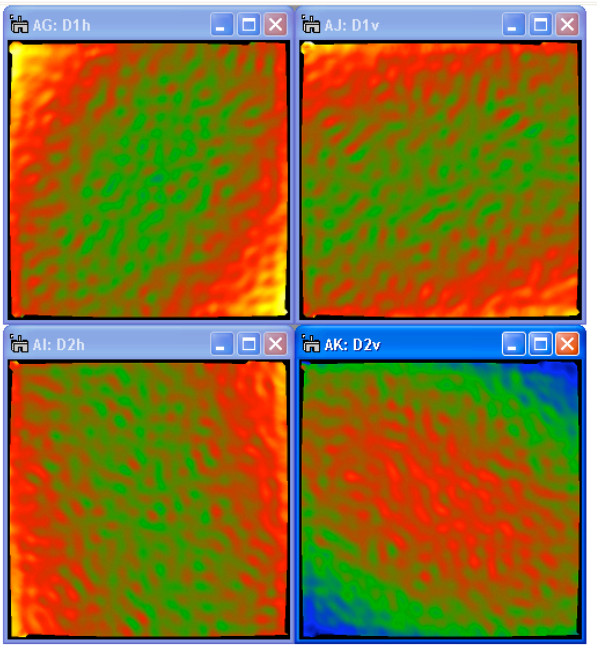
Image rectification

This option allows the user to rectify an image of a perfect crystal, using Peak Pairs information.

Open the image "Substrate.dm3", which corresponds to a perfect crystal image and calculate the *Power Spectrum*.



Bragg-filter the image in the usual way, by selecting three spots in the Power Spectrum and using a custom mask at each spot.

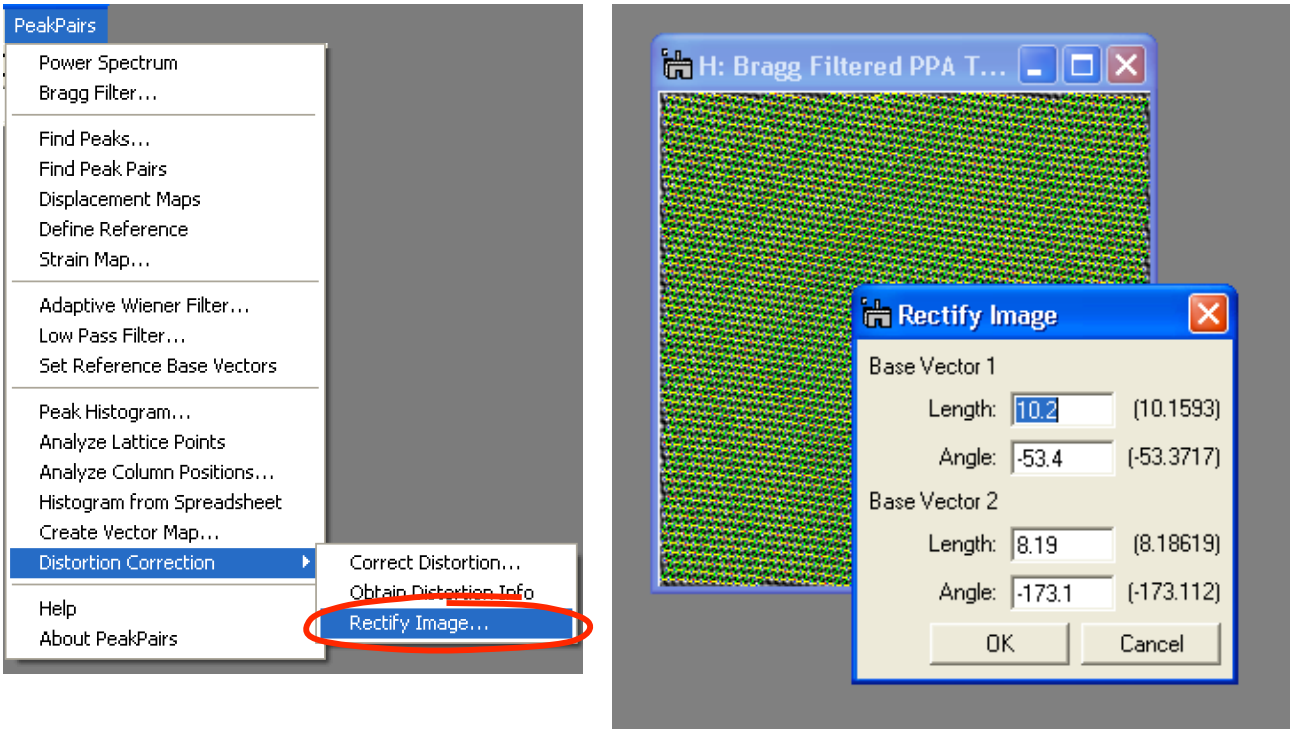


Then calculate the Peak Pairs using the usual commands (*Find Peaks* followed by *Find Peak Pairs*)

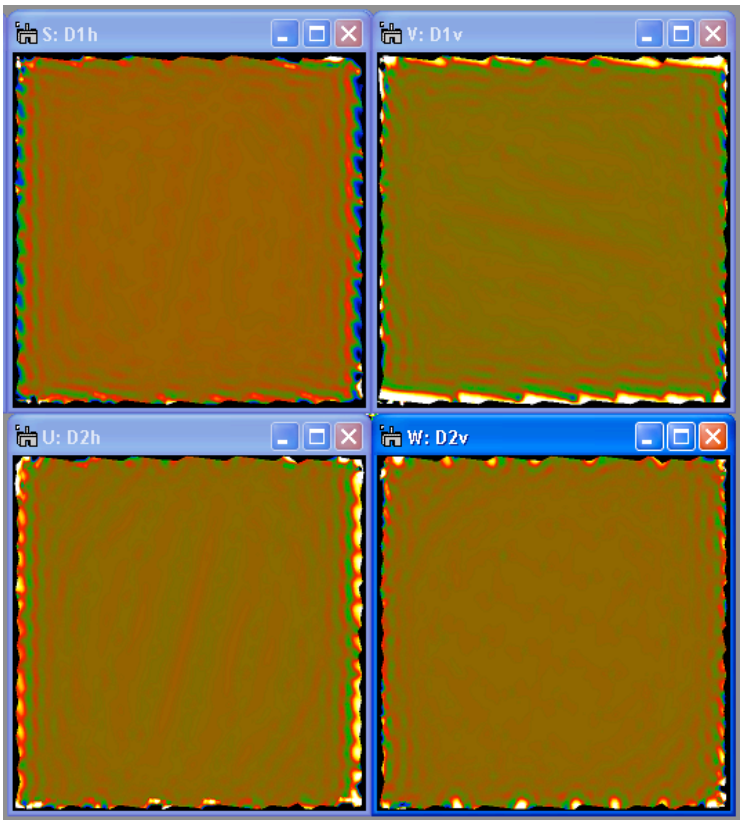
Then calculate the displacements using *Displacement Maps*

The information contained in the resulting displacements is dominated by the geometrical distortions.

Given that the image corresponds to a perfect crystal, we can get a rectified image. In order to do that, just select the Bragg Filtered image and apply the *Rectify image* command.



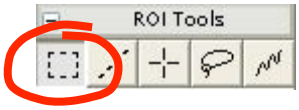
This will produce a rectified image of the perfect crystal using the local distortions at each point of the image. To verify this point, apply a complete analysis process to the rectified image (Power Spectrum-Bragg Filter-Find Peaks-Find Peak Pairs-Displacements Maps), we observe that distortions have been corrected.



Appendix

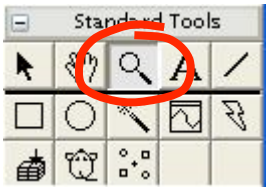
Some useful DM tricks

DM **ROI tool**:



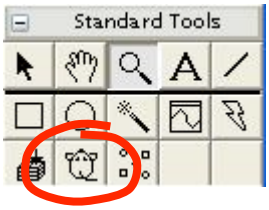
Hint: to select a square area, hold down SHIFT. To select powers of two, hold down SHIFT-ALT.

DM **zoom tool**:



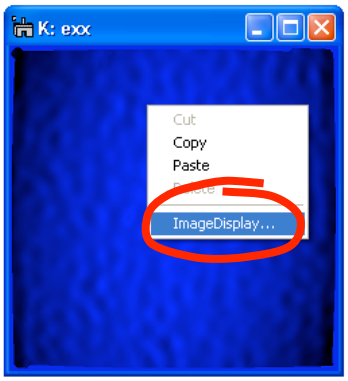
Hint: to demagnify, press ALT.

HREM **Mouse tool**



Hint: to delete any spot, just click on the mouse mark with the SHIFT key down.

DM **Image Display Option**



Hint: to change the color map of any image, press the right mouse button on it, select ImageDisplay, and modify the options as desired.

For example, it is useful to set manually the range of the colormaps to be the same, so as to be able to compare them.