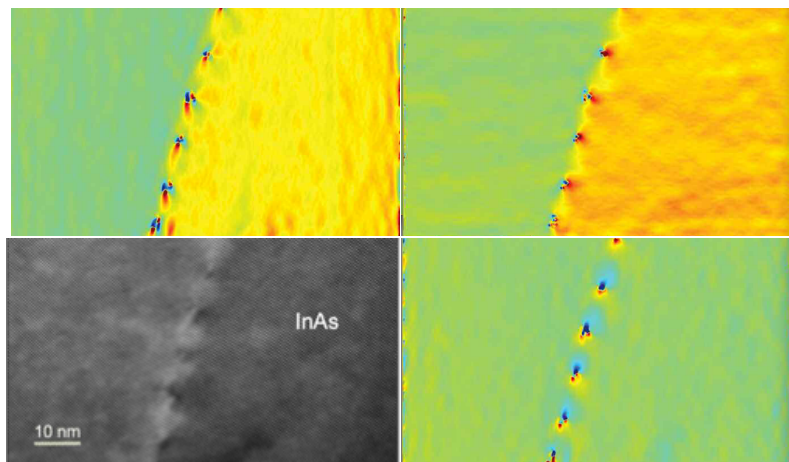


March 2021

PPA for DigitalMicrograph

Peak Pairs Analysis

*High-Resolution Peak Measurement
and Strain Mapping Analysis*



PPA User Manual v4.0

HREM Research Inc.

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DigitalMicrograph is a trademark of Gatan Inc.

Conventions

The typographic conventions used in this manual are described below.

| Convention | Description |
|-------------------|---|
| Bold | Used to denote specified elements 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 select the File Menu and then the Open Option. |
| CAPS | Used to denote the name of a key on the keyboard. For example, the ENTER key. |
| <i>Italics</i> | Used to denote emphasis, captions and the result of an action in a procedure. |

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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 analyzed 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. There is also a quick reference guide at the end of this document.

Software requirements

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

- DigitalMicrograph (Gatan™)
- USB Key Driver
- HREM Mouse Tool Plug-in (freeware downloadable from www.hremresearch.com)
- IPU Plug-in (freeware 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. You can find the key driver installer at the plug-in page on HREM Research web site.

Installing DigitalMicrograph Plug-ins

The DigitalMicrograph Plug-in will be provided as Gatan compiled script file(s) (.gtk) and dynamic link library file(s) (.dll). All these files can be installed by copy-and-paste 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 PlugIns will appear as a new menu or an addition to the standard tools.

Installing Mouse Tools

All the files relating Mouse tool plug-in can be installed by copy-and-paste to the folder “PlugIns.” The Mouse tool will appear as an addition to the standard tools.



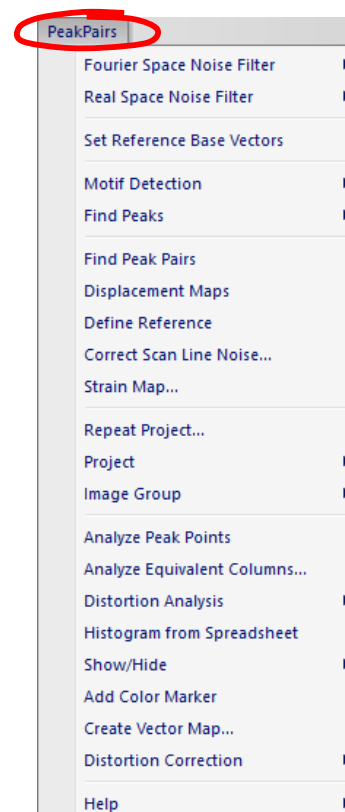
Installing IPU Plug-in

The PPA plug-in 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 copy-and-paste copy. The IPU plug-in will appear as under *IPU* menu. Please consult the ReadMe file that comes with the IPU plug-in.

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.)

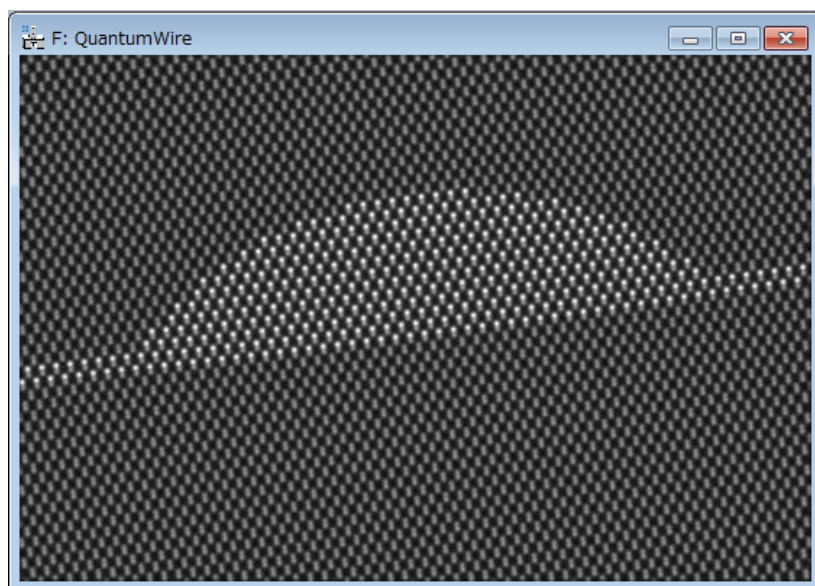
When the DigitalMicrograph is launched after placing the plug-ins into the PlugIns folder, **PeakPairs** menu commands will appear.



Getting Started

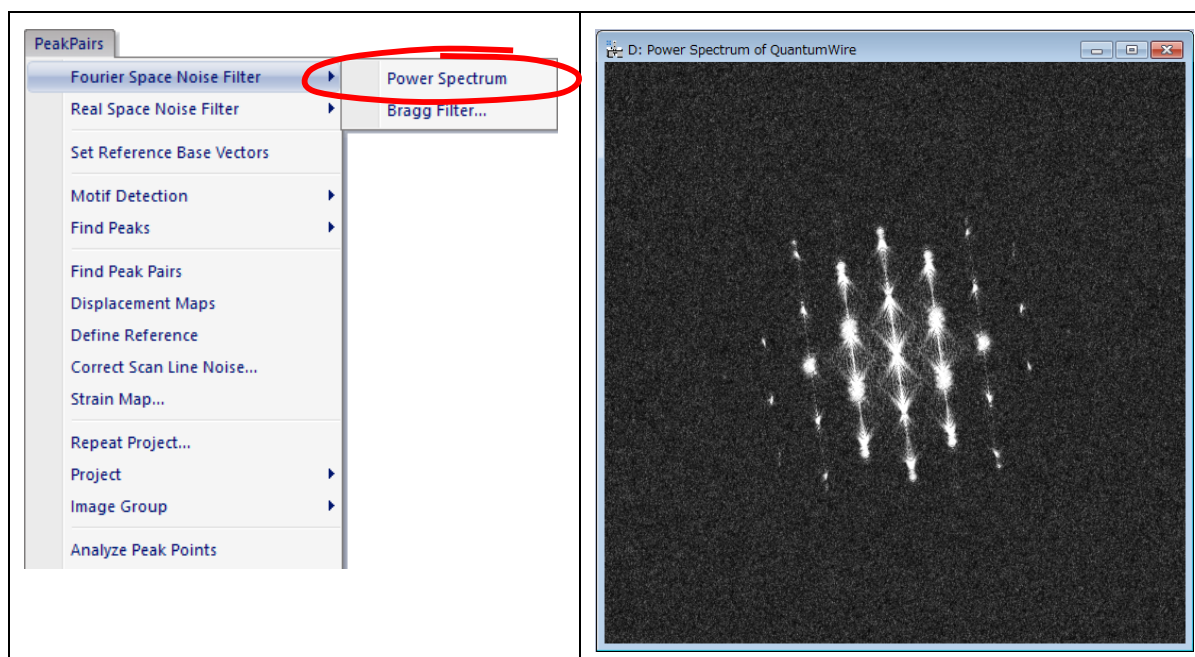
Image pre-processing and Basis Vector Selection (Bragg Filter)

Open the file *QuantumWire.dm3* using the DM command File...Open:

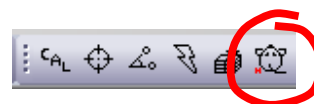


This image represents a capped InAs quantum wire on GaAs. Composition was considered to be uniform inside the quantum wire and across the wetting layer.

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



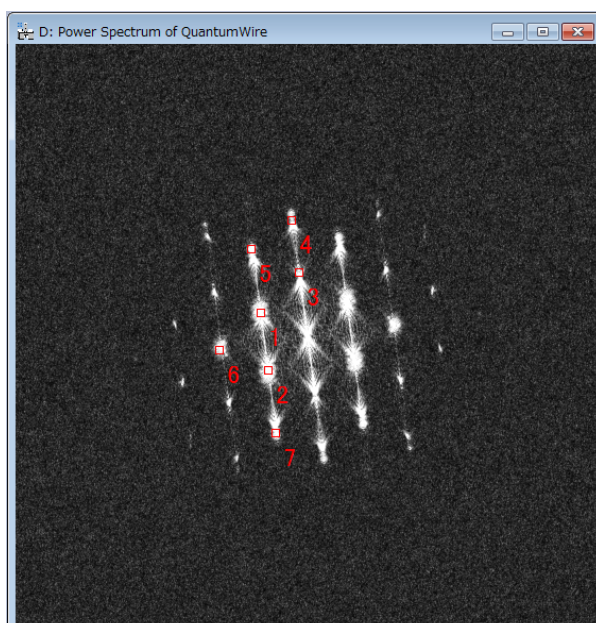
Now, select the **HREM mouse** tool, and click on desired spots to apply Bragg filter. The usual choice is to select the brightest spots in the spectrum, but those corresponding to higher harmonics can also be selected:



The user doesn't need to hit the spot exactly, because PPA looks for the local maxima near the selected point.



Anyway, if necessary, you can zoom in the spectrum before hitting peaks using the **DM zoom** tool:



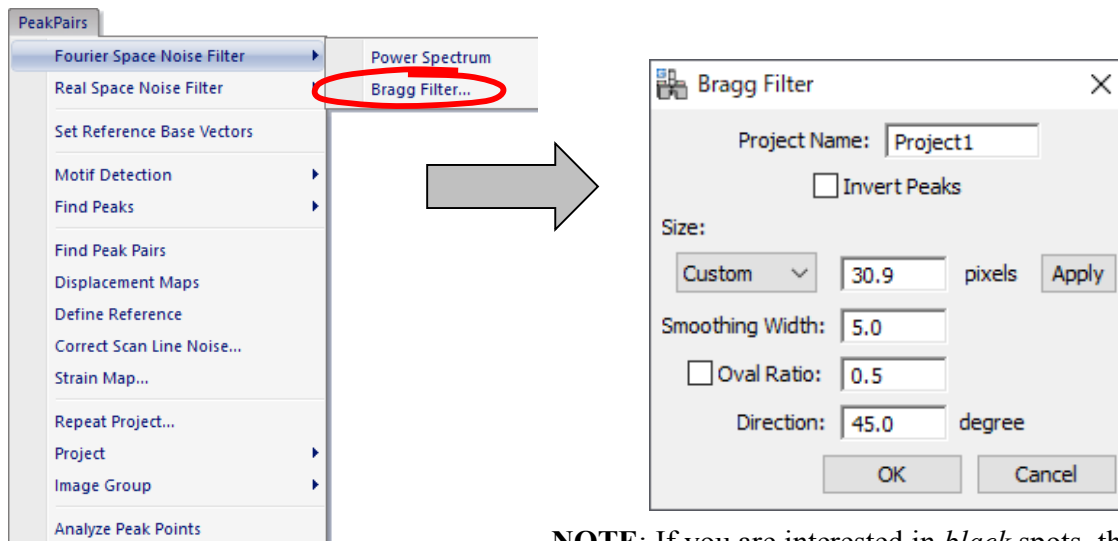
Hint: if you wish to delete any spot, just click on the mouse mark again with the SHIFT key down.

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

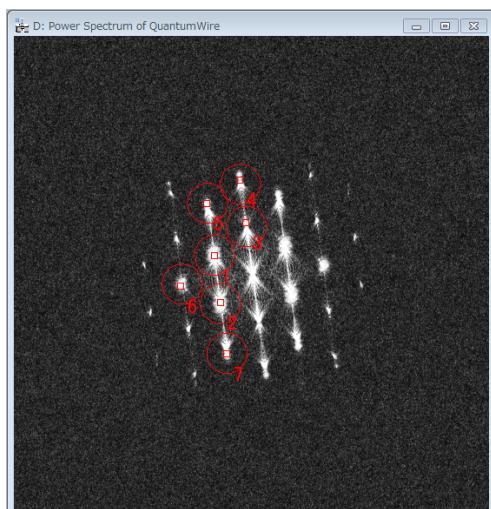
IMPORTANT: *First* and *second* chosen spots (numbered as 1 and 2) will define the lattice basis vectors. These spots should be apart from the vertical or horizontal of the central spot, in order to obtain maximum resolution.

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 **Bragg Filter**. This process creates an image where the contrast resulting from the ordered regions is clearly distinguishable from the background intensity.

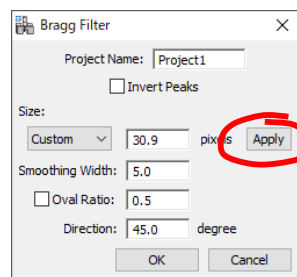


NOTE: If you are interested in *black* spots, the **Invert Peaks** will be checked here.



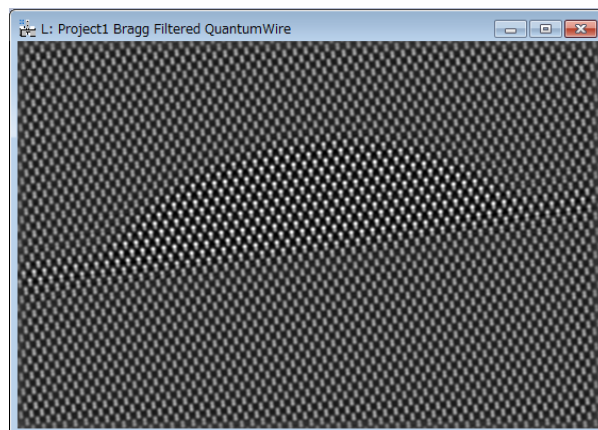
The shape and size of the Bragg filter must be adjusted such that no loss of information occurs. In this dialog box we can determine the size (in pixels), smoothing width (in pixels), oval ratio (height/width) and direction (in degrees) of mask spots.

By pressing the **Apply** button, the mask described by the chosen parameters will be redrawn, as it is shown in the example on the left.



Let us select the first option (small window, oval ratio=1) and press 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 noise.



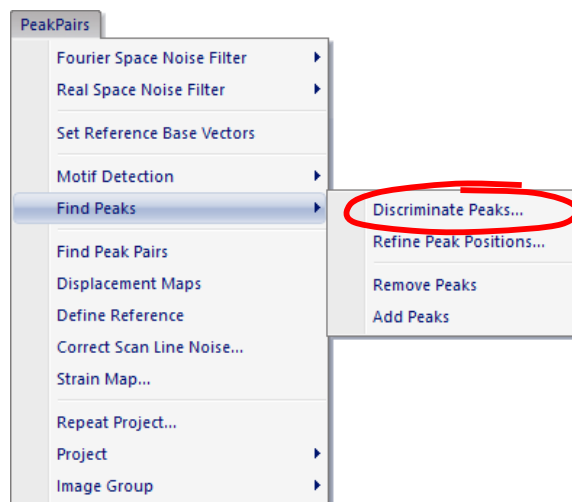
Peak Detection (for simple structure images)

IMPORTANT: Peak Detection uses two base vectors information (unit cell) to find a set of good intensity peaks. The Bragg filter defines the two base vectors automatically. However, in the case of the **Real Space Noise Filter**, the two base vectors should be defined manually using the **Set Reference Base vectors** command.

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

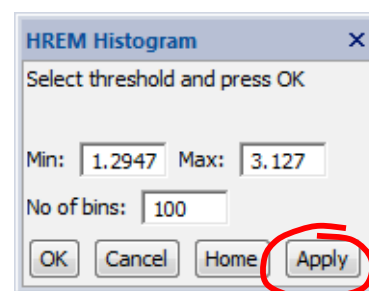
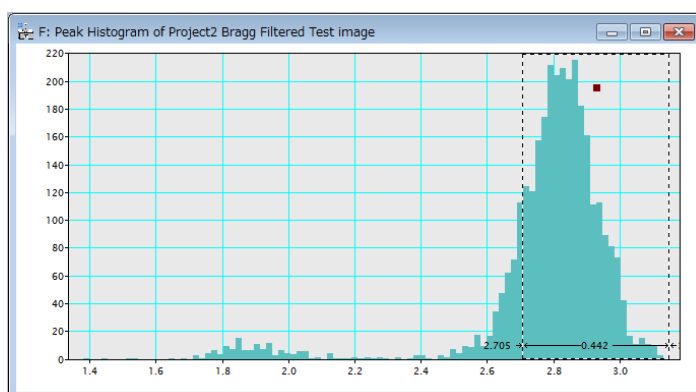
The first step of peak detection is peak identification based on their intensities.

The **Discriminate Peaks** command detects all local intensity maxima in the image, and calculates the histogram of peak intensities.



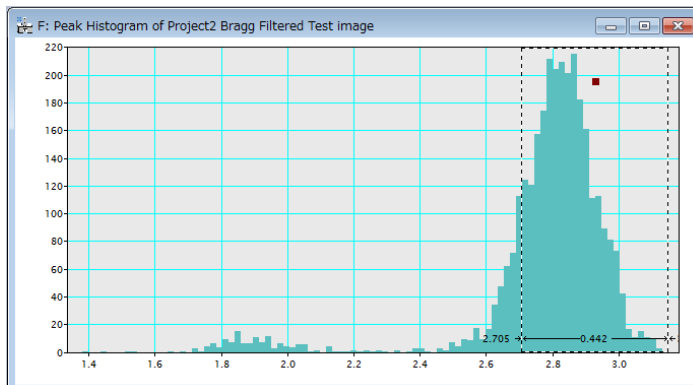
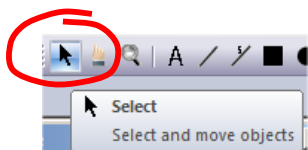
Here, we use *Test image.dm3* as a sample data. First, we apply the Bragg filter using all the spots in the Power Spectrum. When the command **Discriminate Peaks** is selected, a new window showing the histogram of all the peaks found in the image will appear. The histogram allows the user to locate different sets of peaks, based on their intensities. All peaks of intensity lower than this threshold are discarded.

The **Discriminate Peaks** will also open the HREM Histogram control tool. If you want, you can change the histogram range as well as the number of bins. The default range of the histogram is set to the maximum and minimum of the peaks. When you change these values, push the “Apply” button.

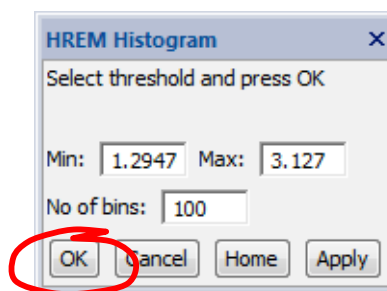
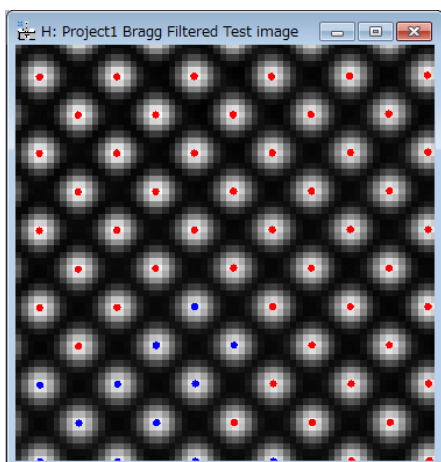


TIPS: If you want to analyse *black* spots (hollows or dips), you have to check **Invert Peaks** when you create a project.

Once the histogram is shown, the user should select the intensity threshold for identifying which peaks will be used in further analysis. To do so, just click the mouse on the histogram, and select the desired range of peaks. The left side of the selection made in the histogram will be used in the following **Refine Peak Positions** command.

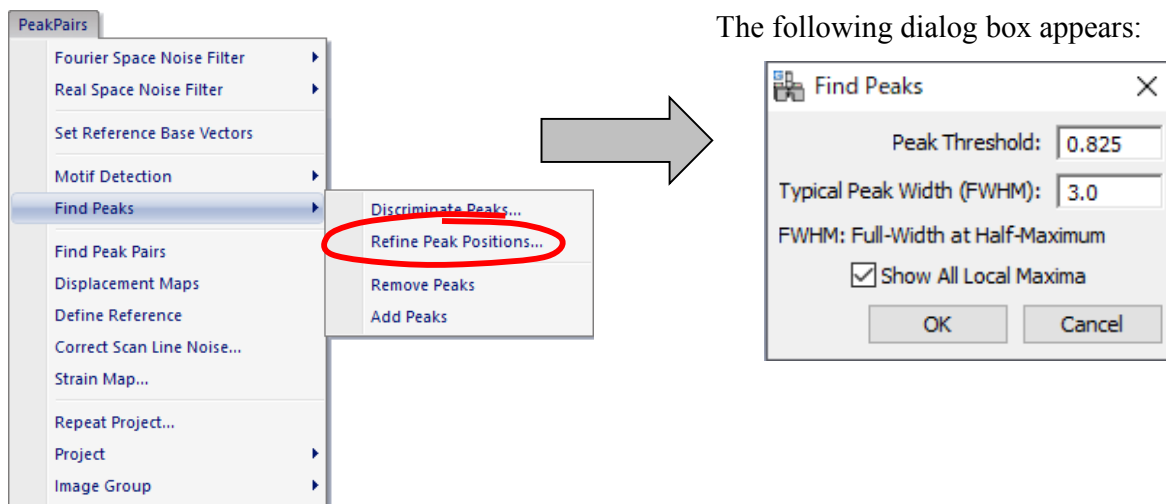


The discovered peaks will be classified to red or blue depending on the peak values: red indicate the peak that is higher value than the selected threshold, while blue indicate the peak equal to or lower than the threshold. The peak colour will be dynamically revised by changing the threshold (the left-edge of the Range ROI).



When you satisfy the threshold by looking the motif markers (red or blue), push the “OK” button of the Histogram tool, or the “Cancel” button to stop the process.

Once the range of peaks is selected, the next step is to refine the peak positions using the **Refine Peak Positions**.

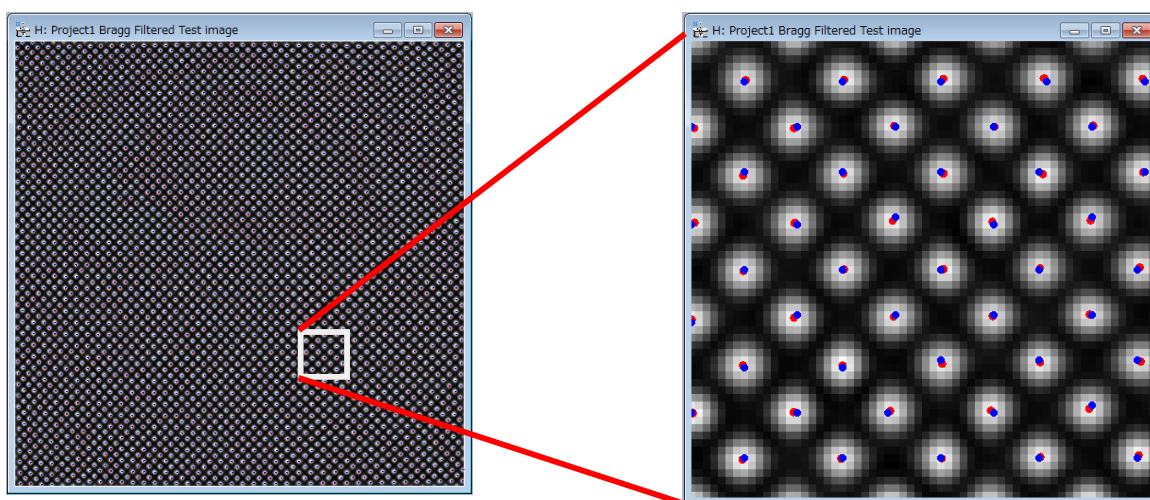


Peak Threshold indicates the minimum intensity of a point to be considered as a valid peak. Peak threshold value is automatically read from the left side of the selection made in the histogram. However, the user can manually modify this value, if necessary.

Typical Peak Width indicates the size (FWHM) of the typical peak in pixels. The peaks (columns) within this value will be merged into a single peak.

When **Show All Local Maxima** is checked, all the peaks at the local maxima is also displayed in blue in addition the refined peaks (in red).

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 sub-pixel resolution. Sub-pixel resolution is achieved by fitting a 2D quadratic function and calculating the maxima, as described in the reference for the algorithm in the Introduction section.



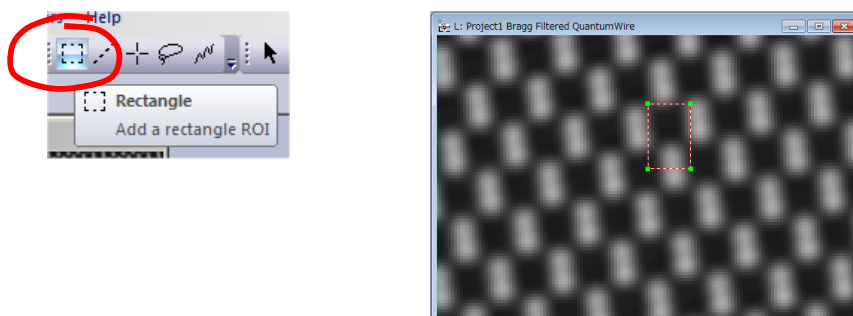
Sometimes, extra peaks are obtained in this automatic Peak Finding process, especially at the borders of the image. Repeating the **Find Peaks** command with a new **Peak Threshold**, all peaks in the border of the image will be discarded and won't be considered in any further calculations.

Motif Detection (for complex structure images)

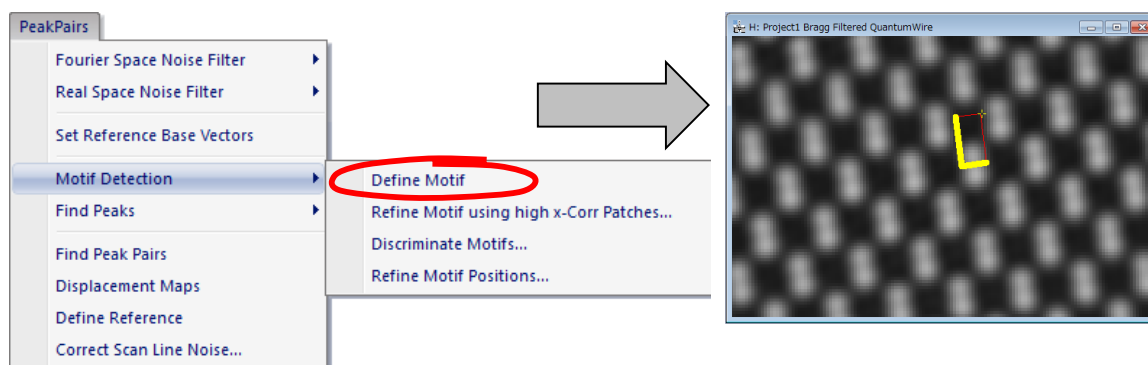
IMPORTANT: Motif Detection uses two base vectors information (unit cell) to find a set of good motifs. Thus, the two base vectors should be defined manually using the **Set Reference Base vectors** command. At this point, a new project will be created.

In cases where the repeating unit in the image is more complex than a single dot, such as a dumbbell, an alternative, more complex way to determine the lattice may be useful. Thus, the **Motif Detection** has been implemented. Here, we explain the Motif detection using the image *QuantumWire.dm3*.

First, a rectangle should be defined using the **Rectangle ROI** tool. The rectangle defines the basic pattern that will be searched across the whole image using normalized cross-correlation. For example, in this image, a cation location (an upper part of a dumbbell) may be a good choice. Rectangle size and location is a critical decision in the accuracy of strain results. Let us zoom in the substrate, and select a rectangle area around a cation.

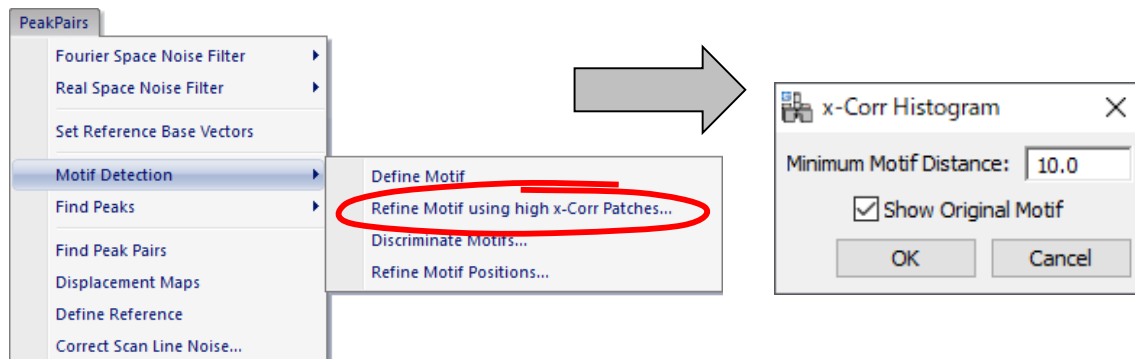


Once the rectangle ROI has been placed, you can rotate the Motif ROI, if you want. To do so, please select the **Define motif** in the Motif Detection submenu.

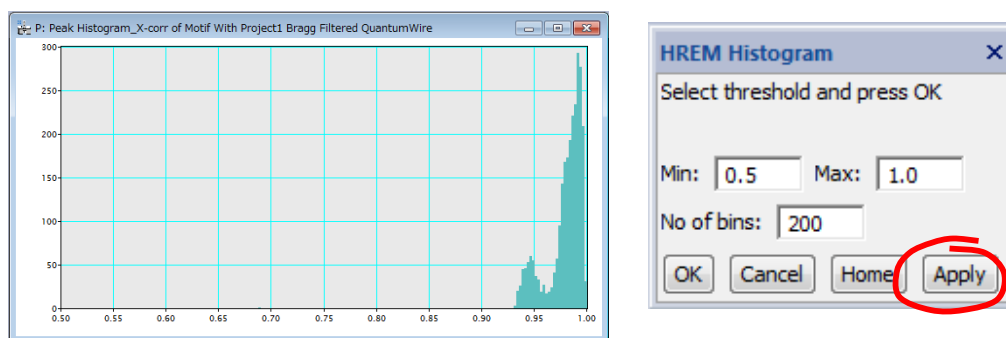


TIPS: You can *rotate* the ROI by dragging the yellow cross (+). You can adjust one of the edge lengths by selecting the yellow edge and dragging the handle. You can adjust both edge lengths by dragging the yellow cross when pressing the SHIFT key

Once the Motif has been defined, select the **Refine Motif using high x-Corr Patches** in the Motif Detection submenu. This command will refine motif using a high score cross-correlation patches with the original motif. When you select this command, a dialog shown below will open:

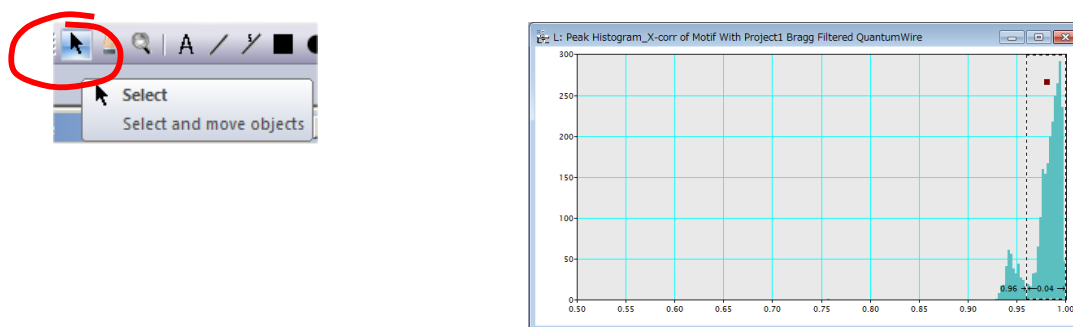


After clicking OK, a new window will appear showing the histogram of all maxima found in the Cross-Correlation map, obtained using the *User-Selected* motif and the whole image. At the same time, the HREM Histogram control tool will appear as shown below.

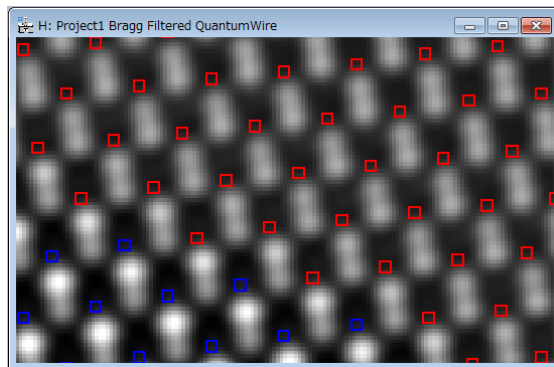


In this case, we may observe two peaks in the histogram, corresponding to Ga and In cations across the image. The default range of the histogram is set to 0.5 to 1.0. If you want, you can change the histogram range as well as the number of bins. When you change these values, push the “Apply” button.

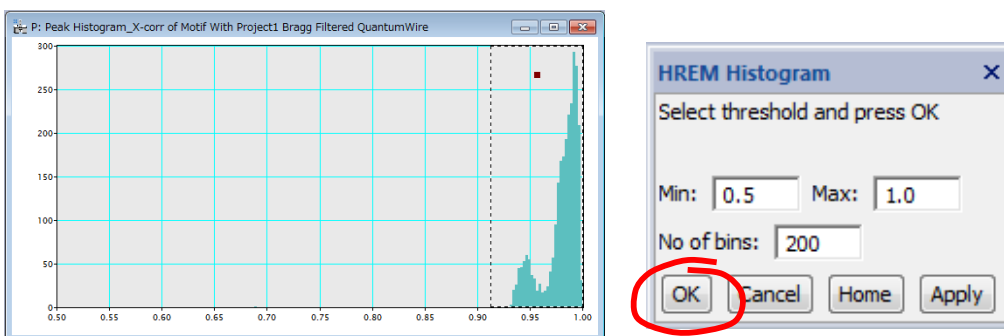
Once the histogram is shown, you should select the intensity threshold for identifying which peaks will be used in further analysis. To do so, choose the **Select** tool and click the mouse on the histogram. Then, move the left edge of the selection to define the lower threshold.



The discovered motifs will be classified to red or blue depending on their cross-correlation values: red indicate the motif, whose cross-correlation value is higher than the selected threshold, while blue indicate the motif equal to or lower than the threshold. The peak color will be dynamically revised by changing the threshold.

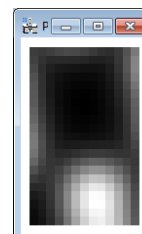


Given that we are interested in the detection of both cations, we will select a threshold lower than 0.9 to take all peaks into consideration.

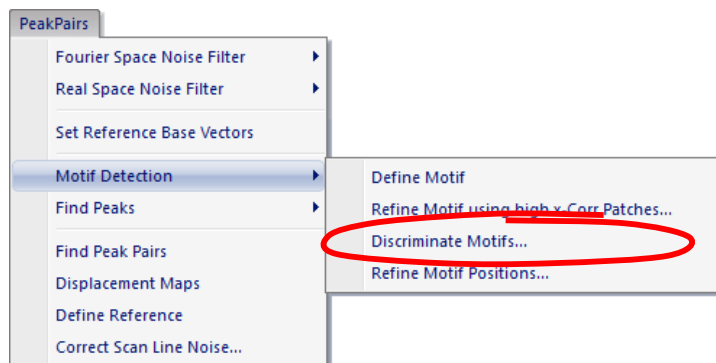


When you satisfy the threshold by looking the motif markers (red or blue), push the “OK” button of the Histogram tool, or the “Cancel” button to stop the process.

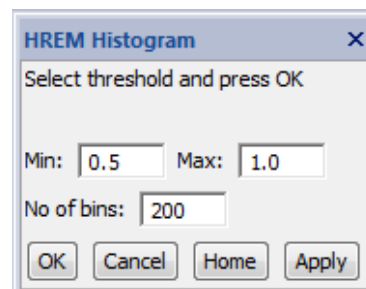
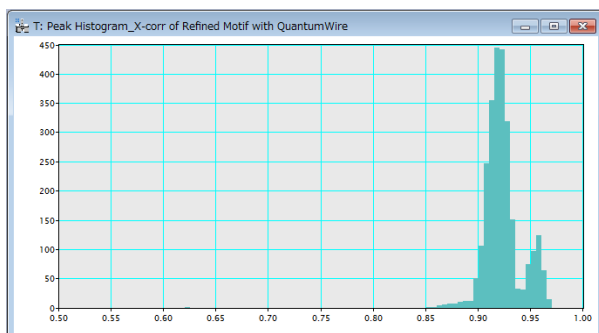
If you push the “OK” button, the first refined motif is calculated by averaging all patterns associated to each point in the histogram above the chosen threshold (0.91 in the figure). The averaged motif is automatically shown:



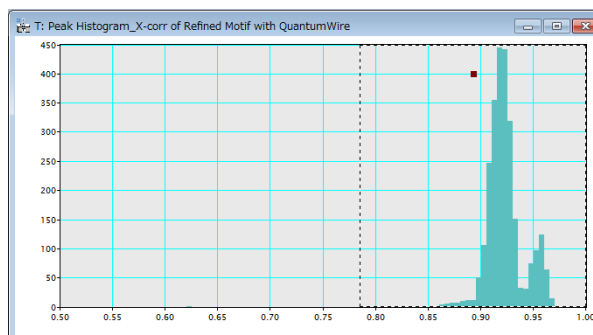
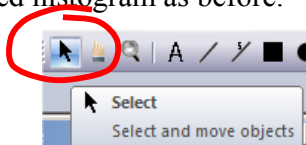
The third step of the Motif detection is calculating the cross-coefficients using the refined motif. To do so, select the Discriminate Motifs command.



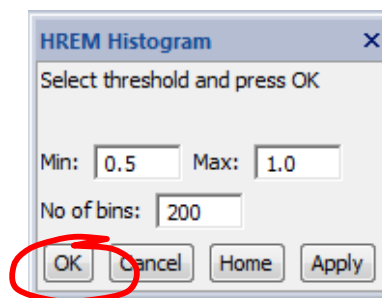
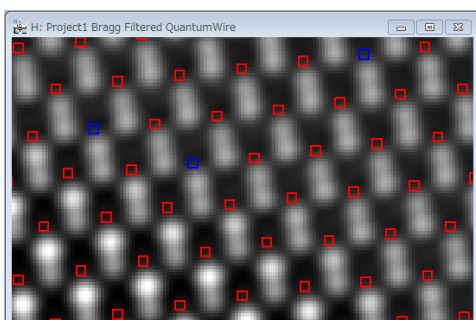
Then, this command will show a histogram of the cross-correlation between the refined Motif and the whole image as well as the HREM Histogram control tool. This step is especially useful in the presence of noise.



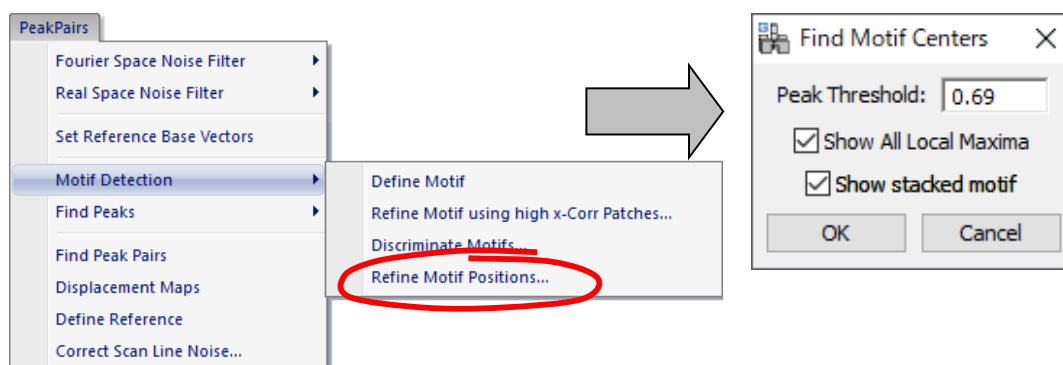
Once the refined histogram is shown, the user should select the intensity threshold on the refined histogram as before.



The discovered motifs will be classified to red or blue as before. The peak colour will be dynamically revised by changing the threshold. When you satisfy the threshold by looking the motif markers (red or blue), push the “OK” button of the Histogram tool.

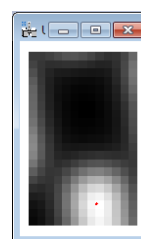
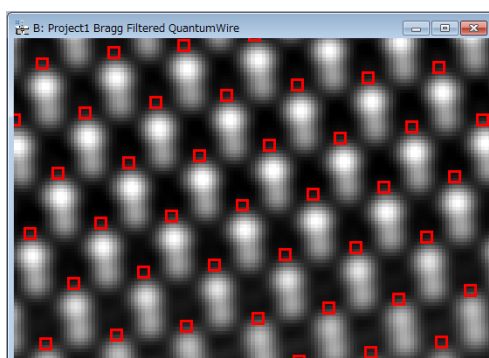


The final step of the Motif detection is finding the refined motif centers (positions) by using quadratic fitting to the cross-correlation peaks. To do so, select the **Refine Motif Positions** in the Motif Detection submenu, which opens the dialog as shown.



If the motif peaks within the minimum motif distance are found, these peaks will be merged into a single peak position.

Then, the refined motif positions (the centers of the motif boxes) are marked by the *red* small boxes, and the second refined motif will be displayed. When **Show All Local Maxima** is checked, all the peaks at the local maxima is also displayed in *blue*. (Here, no blue boxes are shown).



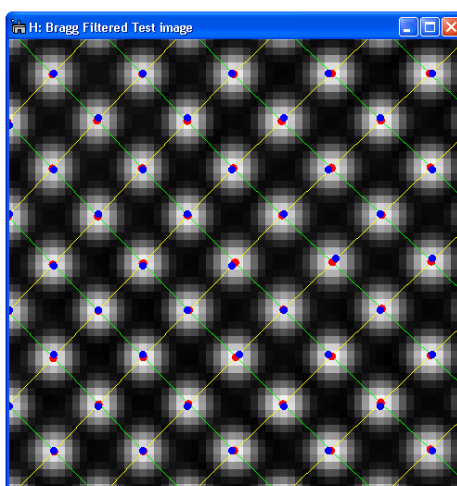
Refined motif

IMPORTANT: In the case of Motif Detection, the reference base vectors should be selected using the **Set Reference Base vectors** before applying the **Find Peak Pairs** command.

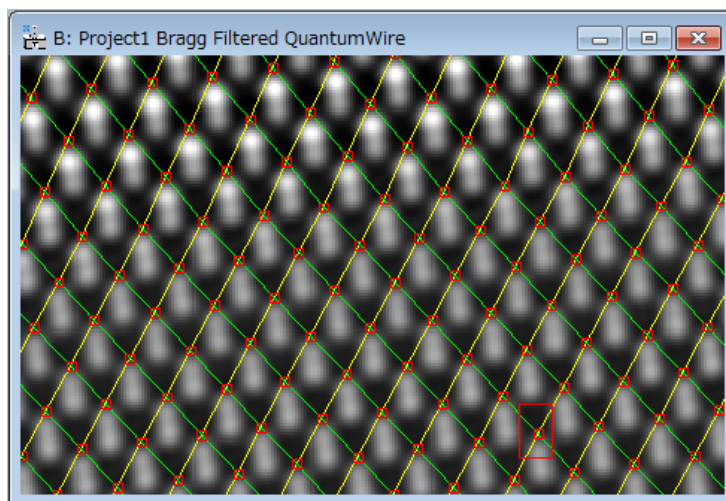
Peak Pairs Determination

IMPORTANT: Peak Pairs are calculated using two basis vectors. The Bragg filter defines the two base vectors automatically. However, in the case of the **Real Space Noise Filter** or **Motif Detection**, the two base vectors should be defined manually using the **Set Reference Base Vectors** command.

Once all peaks or motif centers have been selected, Peak Pairs should be calculated using the **Find Peak Pairs** command. This process will find all pairs of peaks along the predefined two basis vectors.



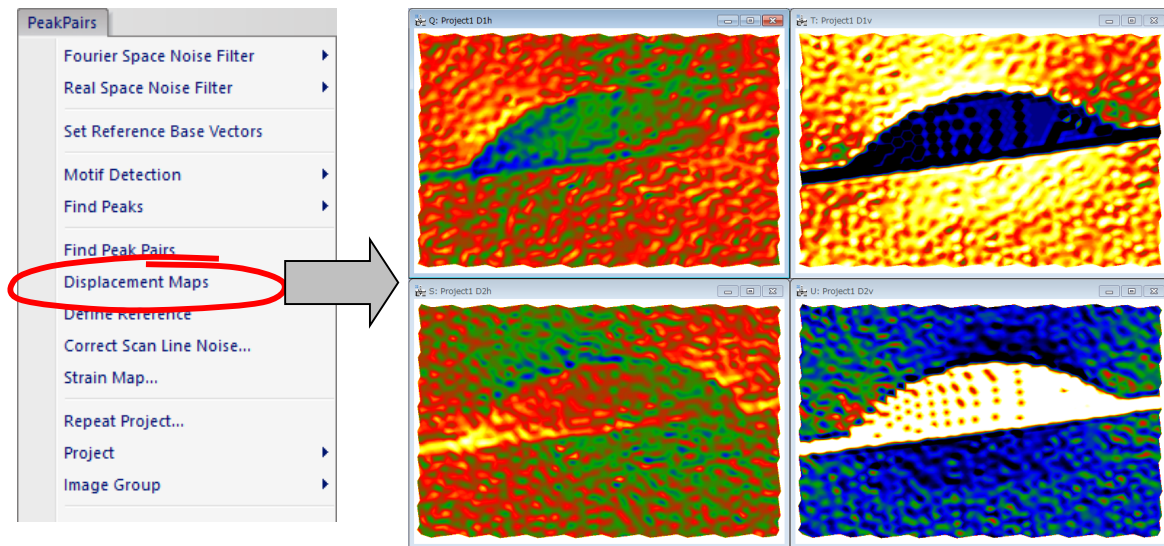
Peak Detection (simple structure)



Motif Detection (complex structure)

Displacement and Strain Maps calculation

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 (D1h, D1v, D2h and D2v).



Technical note:

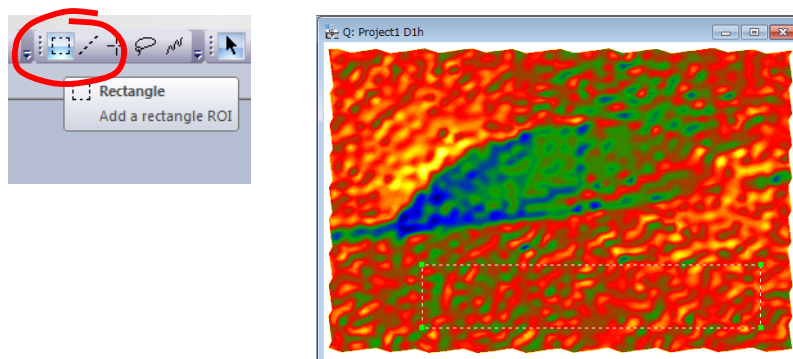
PPA uses an automatic selection of contrast and the temperature color scale for displaying image values. Default color range is ± 1 pixel.

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

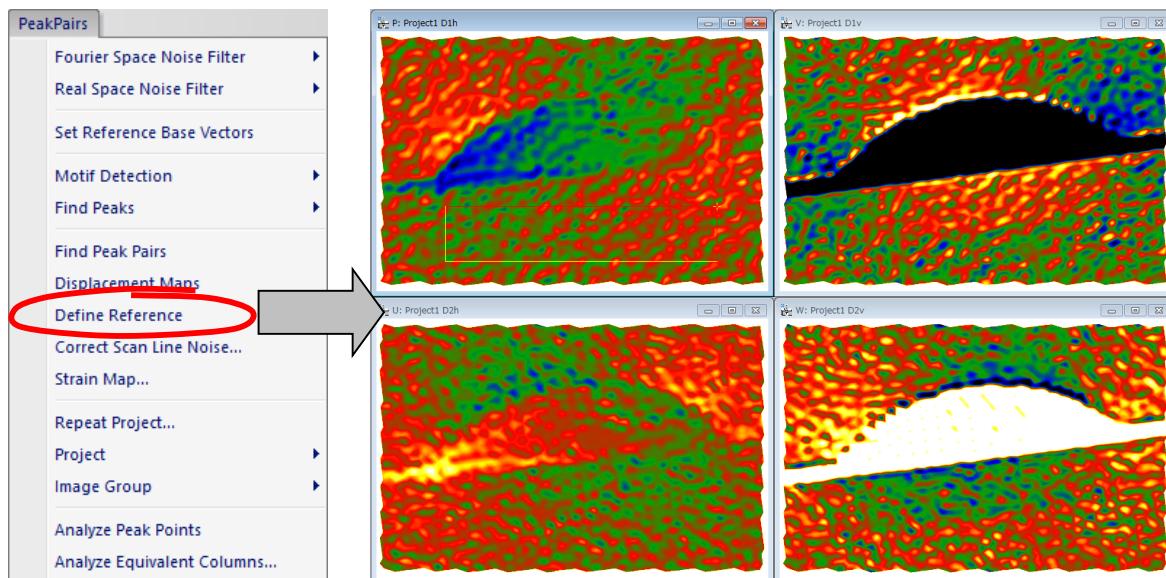
Changing this option will not change the actual values, only its appearance.

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

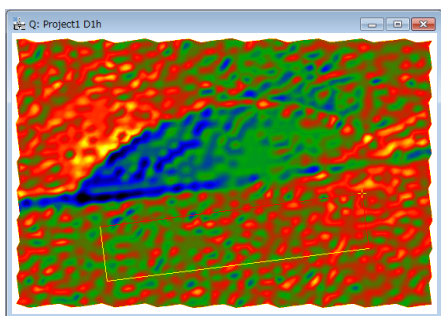
All displacements and strain values will be referred to this area. Use the **Rectangle ROI** tool (region of interest tool) to select an area on any one of the Displacement images (D1h, D1v, D2h or D2v):



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



The **Define Reference** command makes the Rectangle ROI rotatable. You can change the size and angle as shown below, if you want:

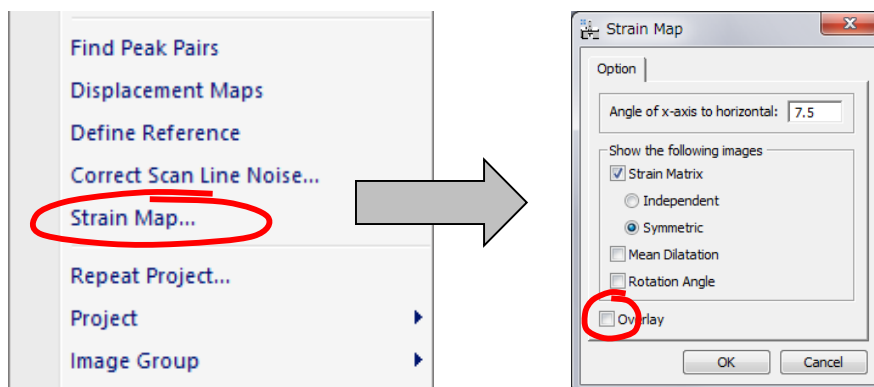


You can adjust the edge length by selecting the yellow edge and dragging the handle, and rotate the ROI by dragging the yellow cross (+).

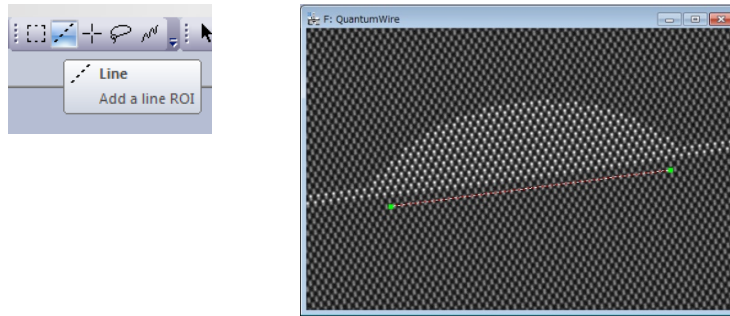
You can adjust the both edge lengths by dragging the yellow cross when pressing the SHIFT key.

When you change the ROI shape or displace the ROI, the average displacement within the ROI will be automatically set to zero.

The final step is the determination of *strain maps* (e_{xx}, e_{yy}, e_{xy} and e_{yx}) at the desired *angle*. When the **Strain Map** command is selected, the Strain Map dialog appears. Here, you can specify the coordinate axes to display the strain maps using **Angle of x-axis to horizontal**. If the angle is set equal to 0, horizontal and vertical directions are assumed to be x and y coordinate axis respectively.



The angle of x-axis to horizontal may be determined graphically. To do so, just add a **Line ROI** on the original image, along the desired direction of x-axis, *before issuing* the **Strain Map** command.



Once the OK button is chosen, a set of 4 images corresponding to $(e_{xx}, e_{yy}, e_{xy}$ and $e_{yx})$ are obtained. The mean dilatation and Rotation angle are additional images available.

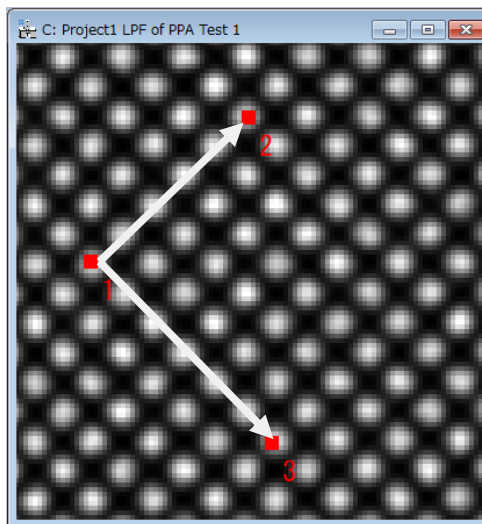
There is an option for strain representation (Overlay):

| <i>DESCRIPTION</i> | <i>Full image</i> | <i>Detail</i> |
|--|---|---|
| <p>No overlay: Continuous strain maps are shown.</p> <p>Hint: If you prefer a grey scale or a different contrast limit, press the right button on the image, and modify ImageDisplay options properly.</p> | <p>A screenshot of a window titled 'K: Project1 exx' showing a full image of a strain map. The image displays a complex pattern of colors (red, yellow, green, blue) representing strain variations across the field of view.</p> | <p>A screenshot of a window titled 'K: Project1 exx' showing a magnified detail of the strain map from the full image. The color variations are more pronounced and detailed.</p> |
| <p>Overlay: Strain maps at each atomic column are shown with colour dots over the original images.</p> | <p>A screenshot of a window titled 'G: Project1 exx' showing the original atomic lattice image with small colored dots overlaid at each atomic column, representing the strain map.</p> | <p>A screenshot of a window titled 'N: Project1 exx' showing a magnified detail of the overlay, where individual atomic columns are clearly visible with colored dots indicating strain at each position.</p> |

Setting the Reference Base Vectors

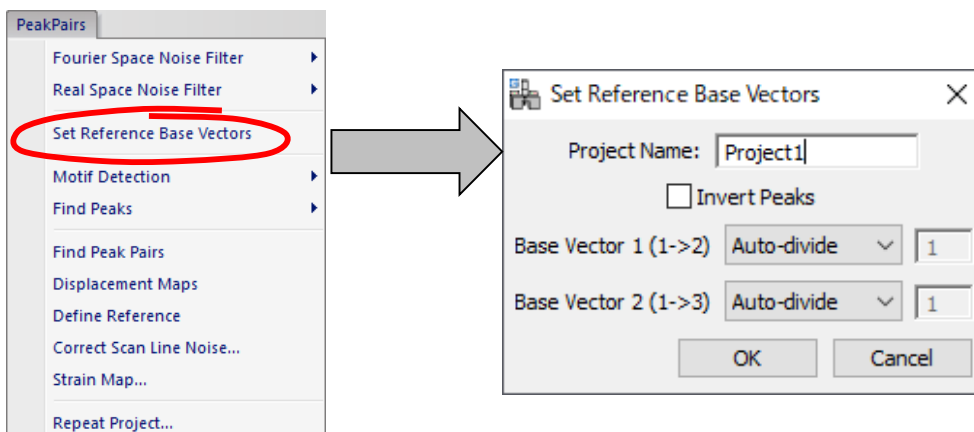
It is possible to manually set the reference base vectors.

To manually define the Reference Base vectors, use the **HREM 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 by the directions of vectors 1->2 and 1->3.



Approximate directions specified by the user

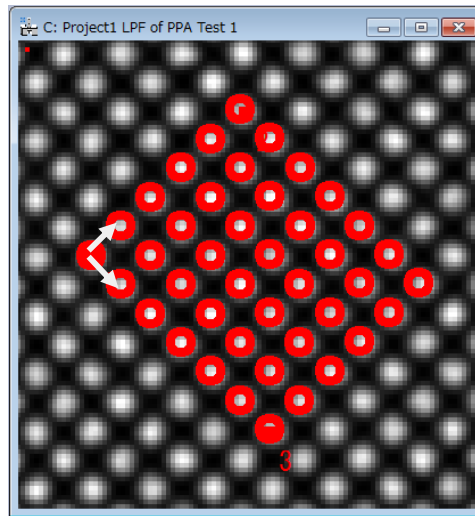
When applying the **Set Reference Base Vectors** command, the dialog shown below will open.



Normally, the reference base vectors along the user specified directions will be automatically estimated. However, if the unit is not simple, the algorithm to determine a repeating unit will fail. In this case, you can specify the number of repeating units along two directions. In this case, 5 and 6 along the base vector directions 1 (1->2) and 2 (1->3), respectively.

NOTE: If you are interested in *black* spots, the **Invert Peaks** will be checked here.

The precise magnitude and direction of both reference base vectors are calculated using a least-squares fitting to all the peaks within the parallelogram defined by two vectors 1- \rightarrow 2 and 1- \rightarrow 3.



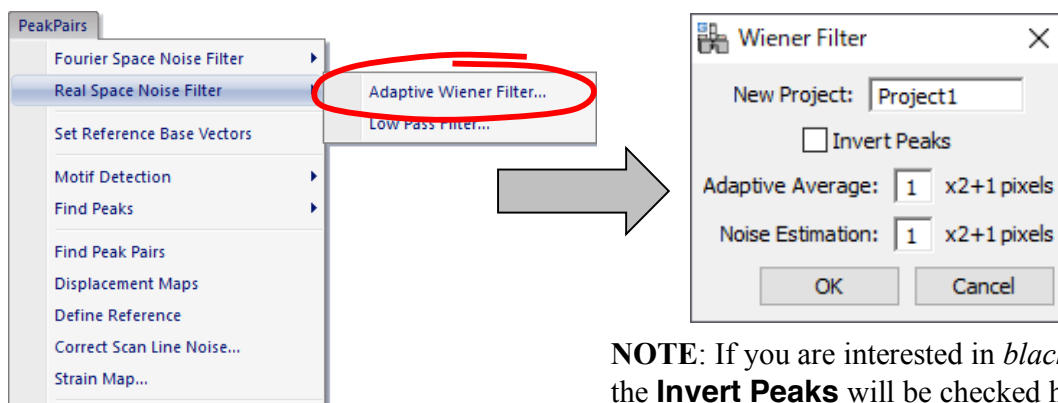
Real Space Noise Filters

While Bragg filtering is very useful to reduce noise, some researchers may prefer other alternative noise filtering techniques in real space. There are two alternative noise filtering commands: **Adaptive Wiener Filter** and **Low Pass Filter**. The techniques have no way to determine automatically the basis vectors, and they should be determined manually by using the **Set Reference Base Vectors** command

Adaptive Wiener Filter

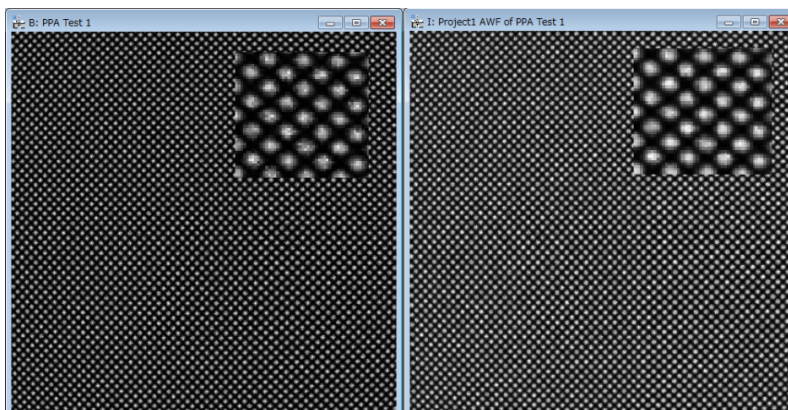
The Wiener filter is widely used for image restoration and calculates the optimal filter for the removal of noise from a signal which is corrupted by the measuring process itself. It assumes that if noise is present in the system, then it is considered to be additive white Gaussian noise.

In a typical Peak Pairs session, if Wiener filtering is desired, it is usually the first operation to be applied to the original image. When applying the **Adaptive Wiener Filter** on the front image, the user should decide the size of the windows used for calculating the **Adaptive Average** and the **Noise Estimation**, as follows:



If the standard deviation of the local area is small, then the pixel value will be replaced by a local average. On the other hand, if the standard deviation of the local area is large, then the pixel value will not be modified. Thus, the new pixel value will be between the old value and the local average according to the local standard deviation.

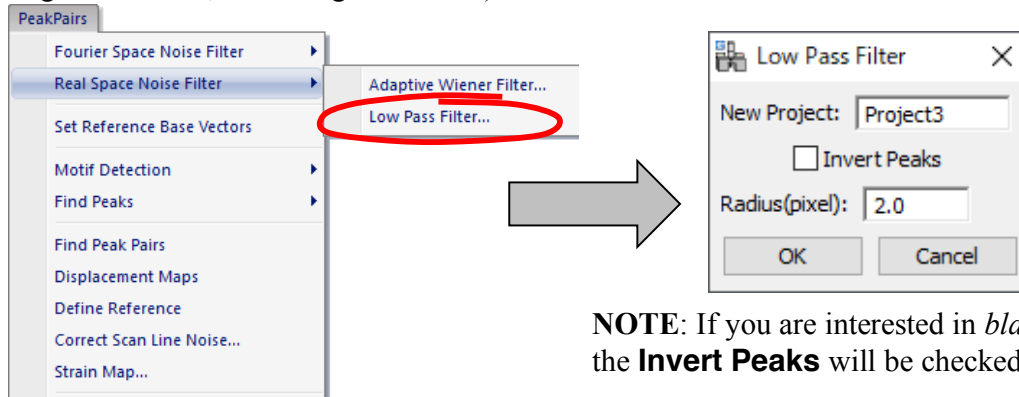
The result of the Wiener filtering applied to *Test image.dm3* is shown below. The insets show enlarged parts.



Left: Original; Right: Wiener (Adaptive Average =3, Noise Estimation=3)

Low Pass Filter

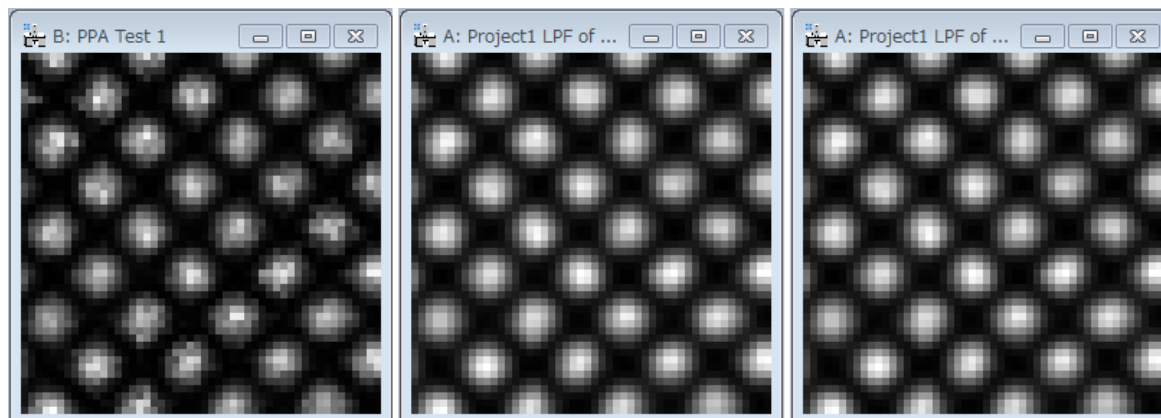
In order to generate a Low-Pass filtered image, use the **Low Pass Filter** command on the front image. The strength of the filter is defined by the Radius of the mask in pixels (the larger the radius, the stronger the filter):



NOTE: If you are interested in *black* spots, the **Invert Peaks** will be checked here.

The new pixel value will be a local average with a Gaussian weight (mask) of the defined radius. You can specify a radius of less than one pixel.

In the following figure, the resulting images after the application of a Low-Pass filter to the lower left part of *Test image.dm3* with different radius are shown:



Original image
(right-lower corner only)

Low Pass Filtered
(radius=0.8 pixels)

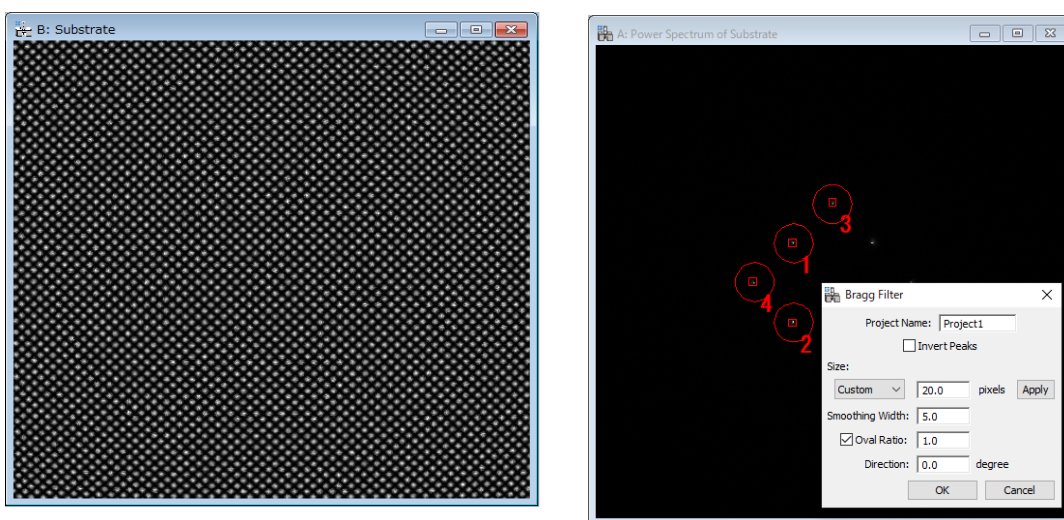
Low Pass Filtered
(radius=1.6 pixels)

Geometric distortion correction

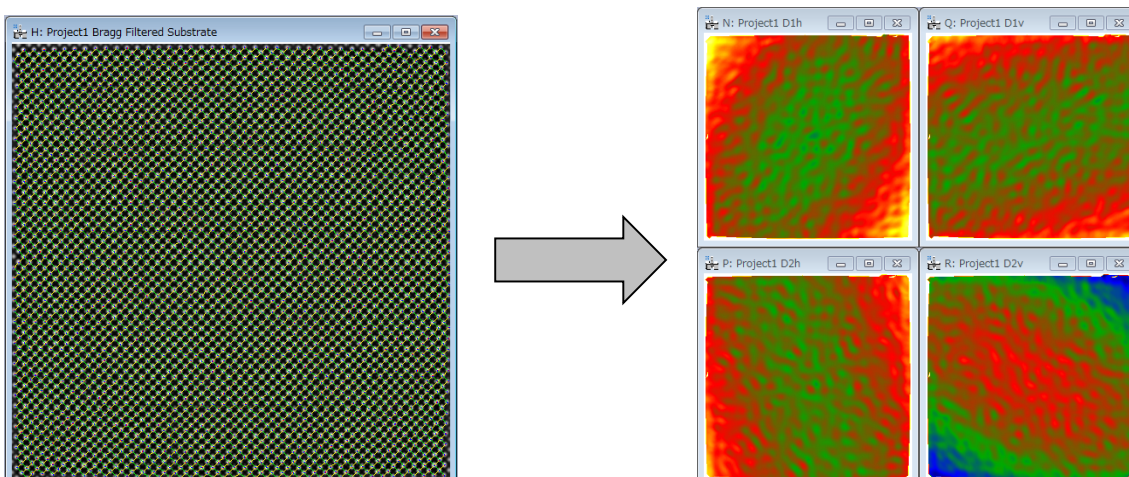
All optical systems distort the images they form. CCD cameras and scanners (for digitising negatives for example) introduce additional distortions. If these geometric distortions are fixed (what is usual for a given system), it is possible to eliminate them. This is valid not only for projector lens 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. We explain here distortion correction using a pair of images with the same distortion, *Test image.dm3* and *Substrate.dm3*, the latter of which corresponds to an image of a perfect crystal.

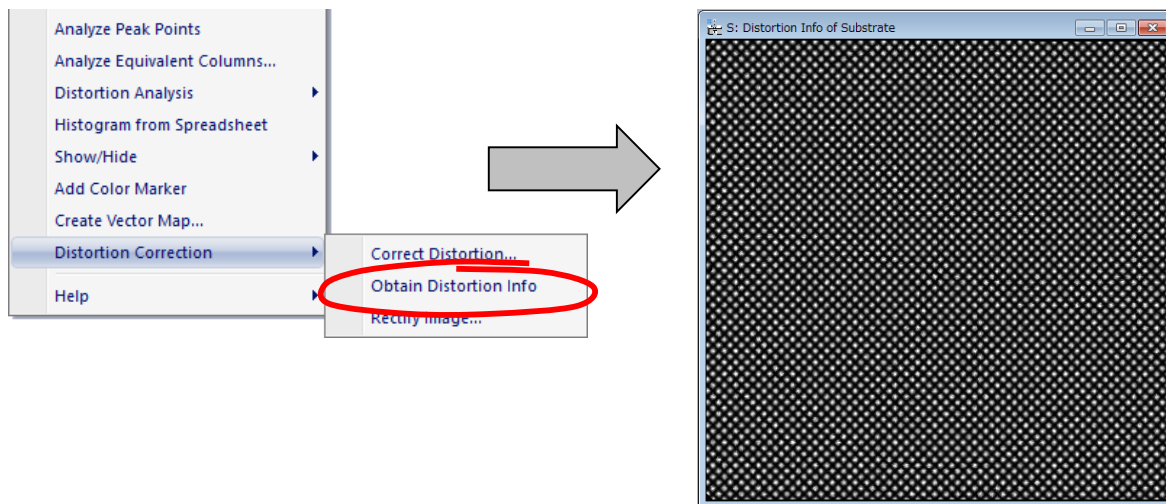
Open the image *Substrate.dm3*, execute the **Power Spectrum**, and then **Bragg Filter** in the usual way by selecting relevant spots in the Power Spectrum.



Then calculate the *Peak Pairs* using the usual commands (**Find Peaks** followed by **Find Peak Pairs**). If we analyse the displacements with the **Displacement Maps** command, we can observe that the image of a perfect crystal is distorted as shown below.

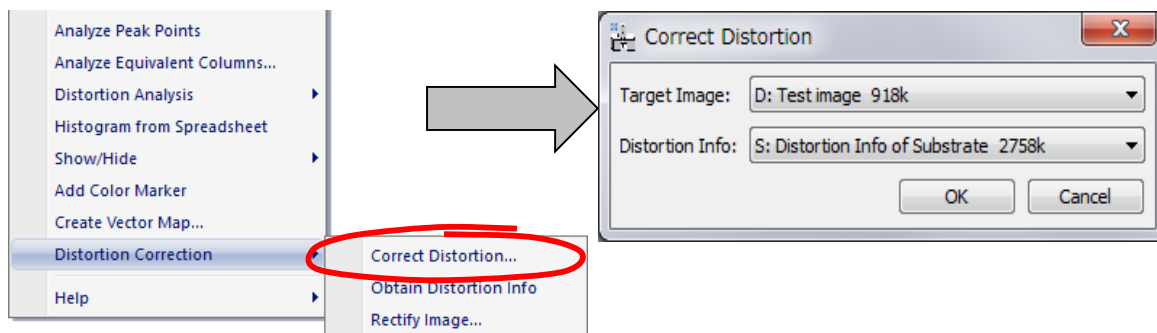


The distortion information obtained for the perfect crystal image can be used to correct distortions in any other image with the same distortion. In order to obtain the distortion information, select the image with *Peak Pairs* information, and apply the command **Obtain Distortion Info**.



The new image with distortion information will be created. This *Distortion Info* image can be saved to disk (e.g., *Distortion Info of Substrate* using **Save As** command) and used in further analysis of the image having the same distortion.

In order to rectify the original image using the distortion information obtained from the perfect crystal image, just apply the **Correct Distortion** on the *Target Image* as follows:

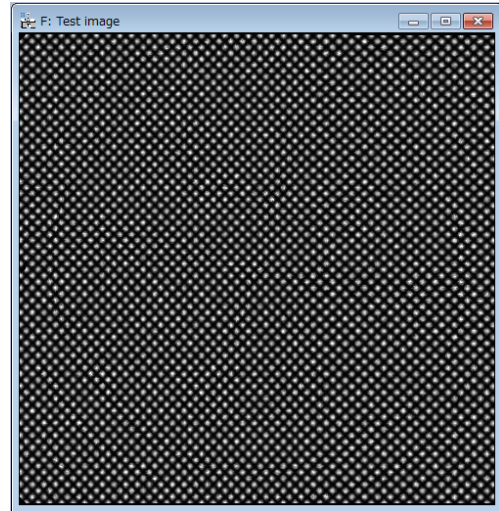


Here, Select the **Target Image** (the image to be corrected), and the **Distortion Info** (the image created by the **Obtain Distortion Info** command). Here, we use the *Test image.dm3* and the Distortion Info obtained from *Substrate.dm3*.

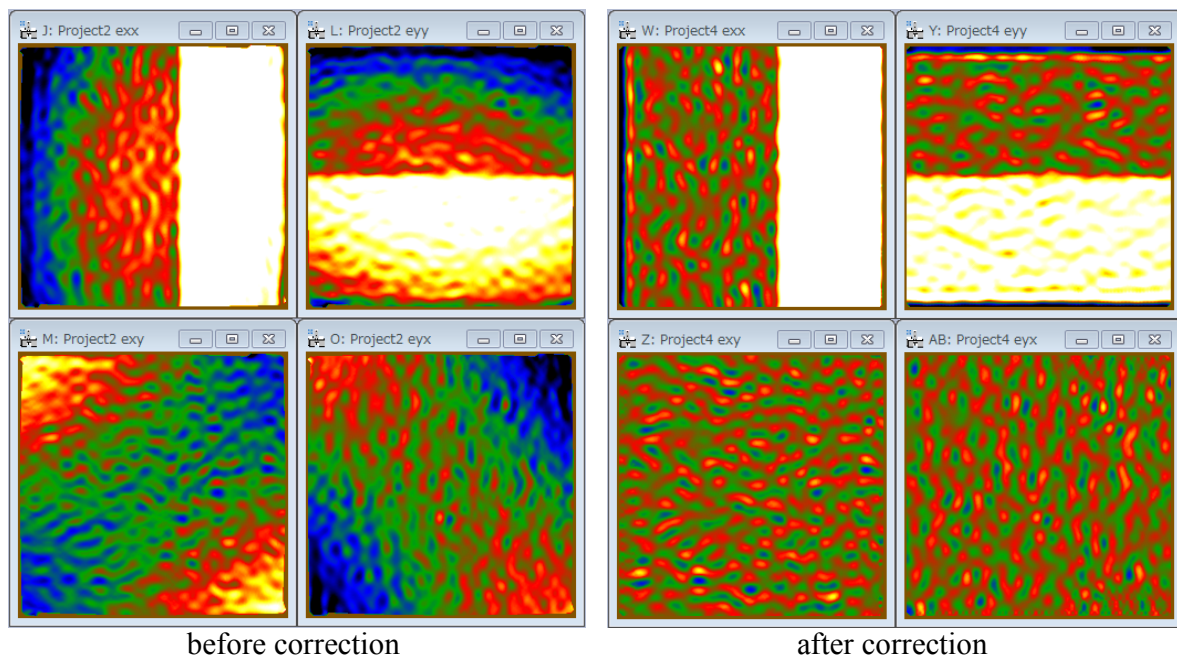
This will produce a corrected image, where all the distortions estimated from the perfect crystal image have been eliminated.

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

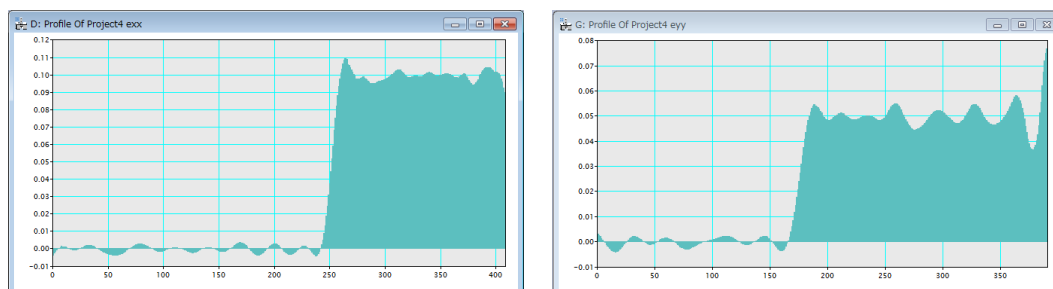
1. Power Spectrum
2. Bragg Filtering
3. Find Peaks
4. Find Peak Pairs
5. Displacement Maps
6. Define reference
7. Strain maps



The strain maps before and after distortion correction:



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

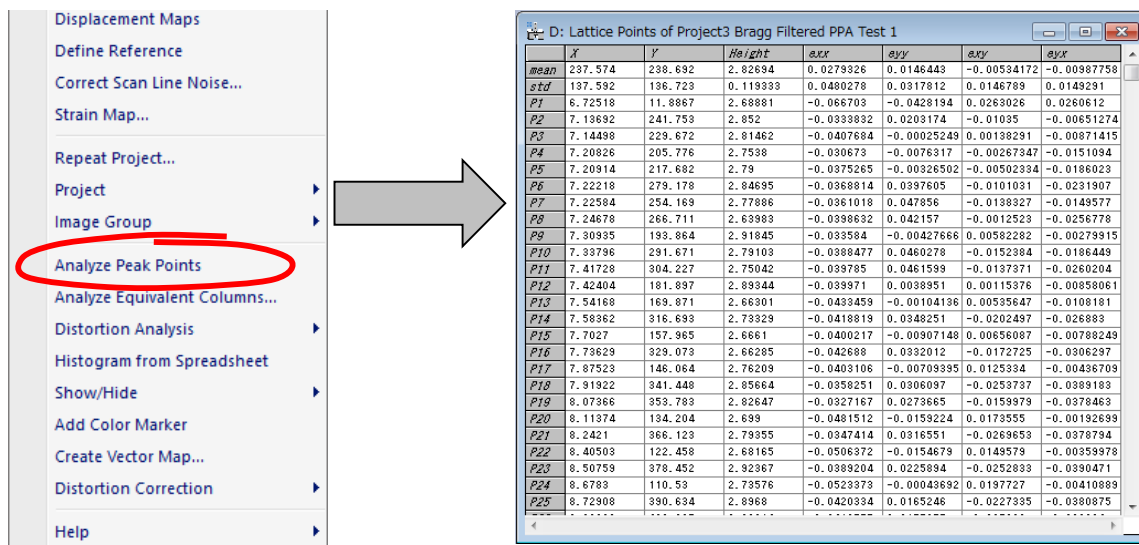


Additional functions

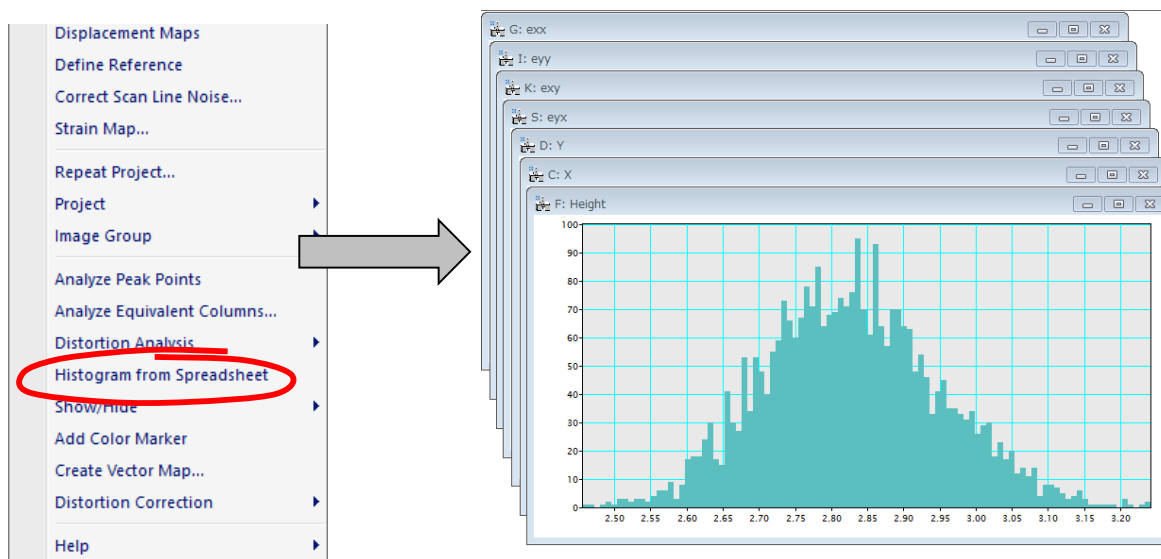
Peak Analysis (Analyze Peak Points)

The **Analyze Peak Points** command applied on the project image, such as Bragg filtered image, will generate an output in spreadsheet including the following information (one row for each lattice peak):

- Peak position at sub-pixel resolution (x,y coordinates)
- Peak intensity
- Strain tensor at each peak points (exx,eyy,exy and eyx): only after Strain Analysis.



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.

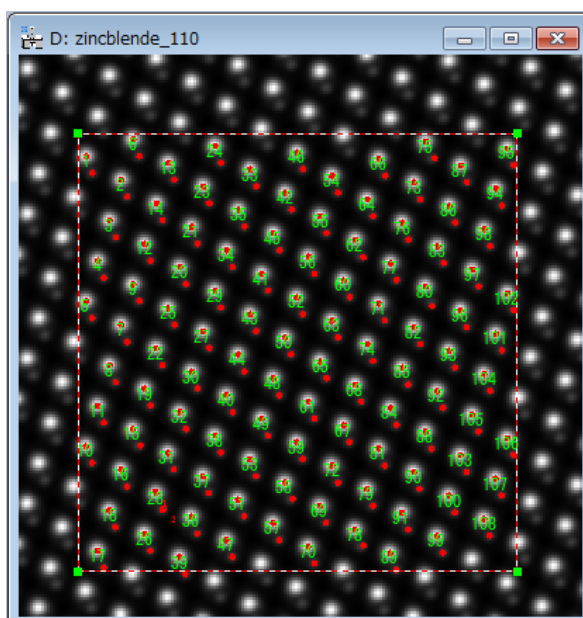
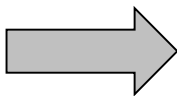
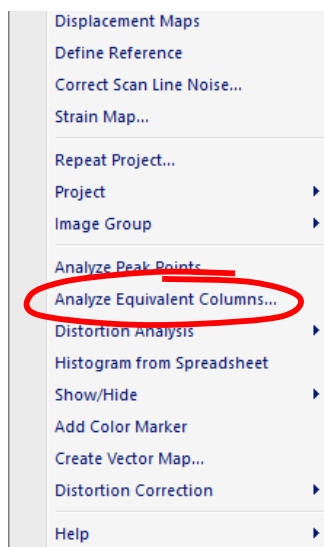
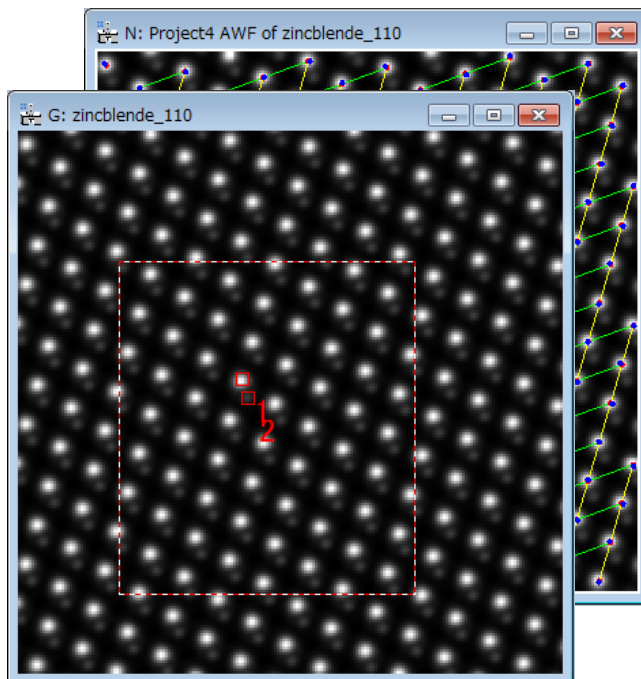


TIPS: When you select this command, a dialog will open, where you can select the data to be displayed.

Atomic Column Analysis (Analyze Equivalent Columns)

Once Peak Pairs have been located, it is possible to analyze atomic column positions. This is very useful when there are more than one atomic column within a unit cell. For example, in the case of [110] projection of InP (the zincblende type materials), we can evaluate cation and/or anion atomic columns. In order to do so, go through the following steps (on the *zincblende.dm3*):

- Calculate Peak Pairs in the usual way
- Bring the original raw image to frontmost.
- Choose the area of interest on the original image using the Rectangle ROI tool.
- Select atomic column(s) to be analysed using the **HREM mouse**. (Here, we select a set of cation and anion columns)
- Bring the project image with Peak Pairs information to frontmost.
- Apply the **Analyze Equivalent Columns** command

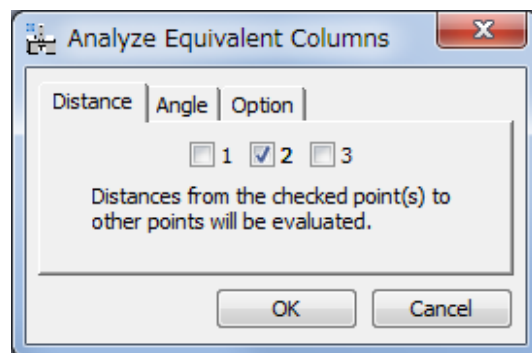


All the columns in the selected area will be shown in the image, and the intensity of each column will be stored in a spreadsheet.

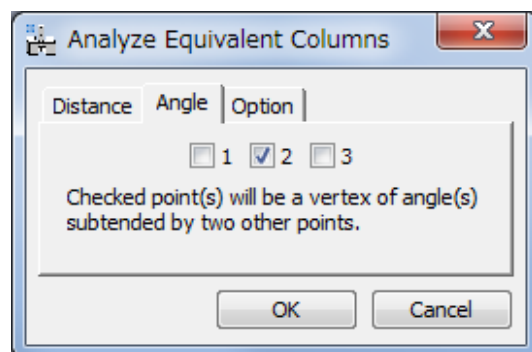
| | 1-2 |
|-------|-----------|
| mean | 6.36442 |
| std | 0.0886919 |
| Pos1 | 6.36691 |
| Pos2 | 6.36616 |
| Pos3 | 6.37164 |
| Pos4 | 6.40395 |
| Pos5 | 6.38842 |
| Pos6 | 6.34961 |
| Pos7 | 6.37638 |
| Pos8 | 6.40828 |
| Pos9 | 6.374 |
| Pos10 | 6.37056 |

| | X1 | Y1 | P1 | X2 | Y2 | P2 |
|-------|---------|---------|------------|---------|---------|-------------|
| mean | 101.92 | 106.428 | 0.306528 | 104.096 | 112.408 | 0.0830263 |
| std | 44.1637 | 44.1373 | 0.00148186 | 44.1625 | 44.1416 | 0.000641297 |
| Pos1 | 35.7585 | 43.9015 | 0.310308 | 37.9353 | 49.8847 | 0.0832183 |
| Pos2 | 31.5959 | 58.2847 | 0.305591 | 33.7563 | 64.273 | 0.0818131 |
| Pos3 | 27.4461 | 72.7096 | 0.30573 | 29.6055 | 78.7041 | 0.0829192 |
| Pos4 | 35.6929 | 95.4985 | 0.304949 | 37.9096 | 101.507 | 0.0836382 |
| Pos5 | 31.543 | 109.836 | 0.307186 | 33.7247 | 115.84 | 0.0841879 |
| Pos6 | 39.8894 | 81.0467 | 0.30447 | 42.0678 | 87.011 | 0.0830656 |
| Pos7 | 27.346 | 124.263 | 0.30509 | 29.5528 | 130.245 | 0.0826102 |
| Pos8 | 44.0382 | 66.6424 | 0.305346 | 46.2168 | 72.669 | 0.0830897 |
| Pos9 | 52.4104 | 37.8367 | 0.306119 | 54.5977 | 43.8237 | 0.0837043 |
| Pos10 | 48.2239 | 52.2539 | 0.305862 | 50.3818 | 58.2479 | 0.0817484 |

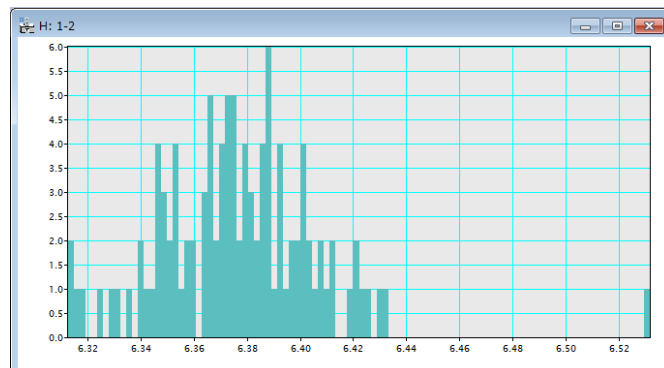
If there is more than one column, the user will have the option to evaluate the distances between the columns.



If there are more than two columns, the user will have the option to evaluate the angles subtended by two neighbour columns.



You can see visually the distribution of distances using the **Histogram from Spreadsheet** command:

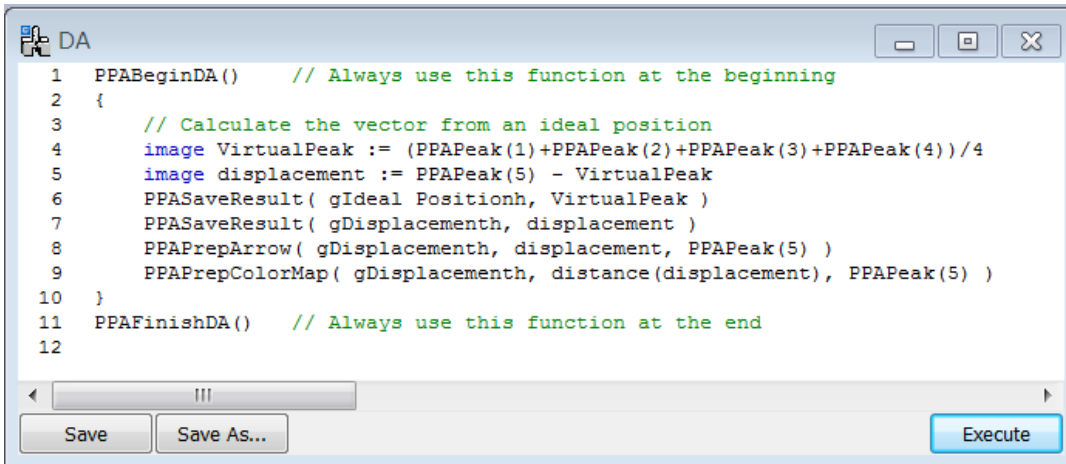


TIPS: When you select **Histogram from Spreadsheet** command, a dialog will open, where you can select the data to be displayed.

Distortion Analysis (from v4.0)

From information on the peak positions of a complex structure, you can analyse a peak distance and angle (a length and angle of the peak-pair vector). Furthermore, in principle, you can calculate a rotation of a structural unit (e.g. tetrahedron or octahedron), or even a distance from the ideal/virtual position to the observed peak. However, such an advanced analysis requires some skill in programming. The Distortion Analysis of the PPA will provide an easy way to perform such an analysis using the DM script.

For the Distortion Analysis we first perform Motif detection, and then on the original image select the peaks to be used in the analysis using the HREM mouse. Next, write a script to measure distortions in the script window as shown below:



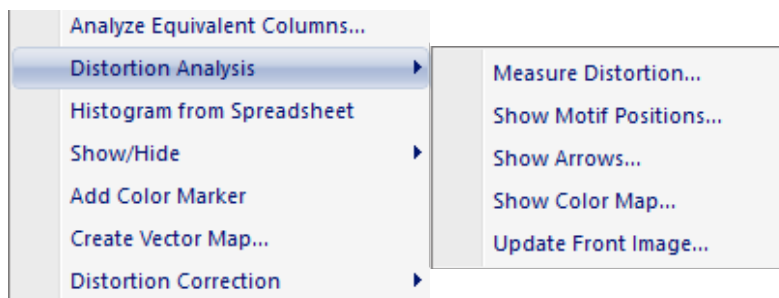
```
1 PPABeginDA() // Always use this function at the beginning
2 {
3     // Calculate the vector from an ideal position
4     image VirtualPeak := (PPAPeak(1)+PPAPeak(2)+PPAPeak(3)+PPAPeak(4))/4
5     image displacement := PPAPeak(5) - VirtualPeak
6     PPASaveResult( gIdeal Positionh, VirtualPeak )
7     PPASaveResult( gDisplacementh, displacement )
8     PPAPrepArrow( gDisplacementh, displacement, PPAPeak(5) )
9     PPAPrepColorMap( gDisplacementh, distance(displacement), PPAPeak(5) )
10 }
11 PPAFinishDA() // Always use this function at the end
12
```

Before executing the script, place a rectangle ROI on the original image to show the area to be analysed. Then, put the project image at the front most, and run the script by pushing “Execute” button. You will get a dialog similar to the one that appears when you select the Measure Distortion command.

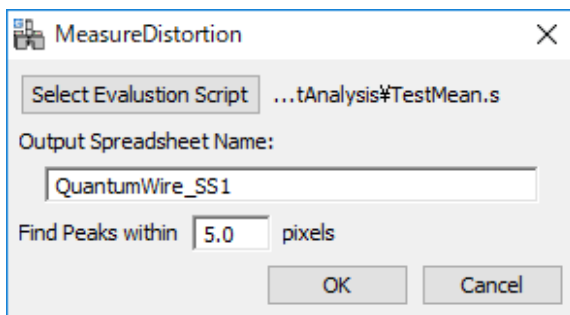
TIPS: If you have no error messages, you may want to save the script for a future use by clicking “Save As...” button. As you see the example script, you have to respectively use PPABeginDA() and PPAFinishDA() at the beginning and the end of the script in addition to your analysing code.

NOTE: This script will measure a distance from the virtual position (the center of the four peaks from peak #1 to peak #4) to the observed peak #5, and save some information for a later use. Here, the functions with the prefix of PPA are provided with the PPA plug-in v4.0 or later and explained at the end of this section.

The following shows the menu for the Distortion Analysis.



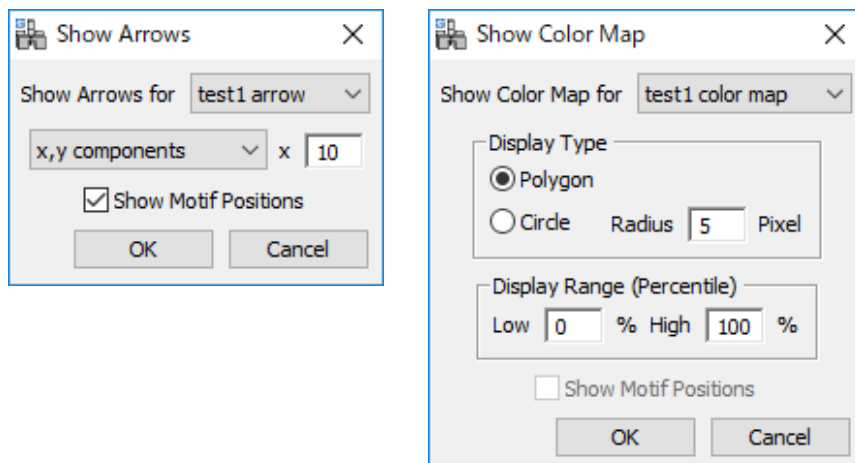
The first step of the Distortion Analysis is to measure distortions by launching the command **Measure Distortion...** to run the saved script, or by directly executing the script from the script window as described above. Before launching the command, place a rectangle ROI on the original image to show the area to be analysed. Furthermore, on the original image select the peaks to be used in the analysis using the HREM mouse. Then, put the project image at the front most, and select the **Measure Distortion** command. This command will open the dialog shown below:



Here, you can select your saved script file to evaluate distortions, and specify the output spreadsheet name. If you directly execute the script from the script window, you will have a dialog without the file selection capability.

Peaks will be searched in the area specified by **Find Peak** within value from the corresponding points in the Motif. If the peak is not found within the specified region, you will find NaN in the spreadsheet.

The measured distortion can be visualized using the commands **Show Arrows...** or **Show Color map...** when the spreadsheet obtained by the analysing script is at the front most. Then, the dialog shown below will open. After selecting one of the spreadsheets, the same dialog will open.



The commands **Show Arrows...** and **Show Color Map...** will work for the spreadsheet that includes the information saved by **PPAPrepArrow** and **PPAPrepColorMap**, respectively.

When the project is at the front most, for which the distortion is measured, the dialog to select a spreadsheet data will open. Then, follow the same steps of showing the arrows or color map.

TIPS: You can modify the appearance of the map using the **Update Front Image...** command, if the front-most image is an arrow or color map.

You can check the potions of the approximate motif centres using the **Show Motif Positions...** command.

Description of the functions

PPABeginDA()

should be called at the beginning of the script

PPAFinishDA()

should be called at the end of the script

image PPAPeak(number n)

generates a list of column positions for the peak #n.

image PPALength(image vector)

calculates the vector length.

image PPALength(image point1, image point2)

calculates the length of the vector (point1 to point2).

image PPAAngle(image vector)

calculates the vector angle, anticlockwise from the horizontal axis.

image PPAAngle(image point1, image point2)

calculates the angle of the vector (point1 to point2), anticlockwise from the horizontal axis.

image PPAAngle(image point1, image point2, image point3)

calculates the angle between two vectors (point1 to point2, and point1 to point3), anticlockwise measured from point2 to point3.

void PPASaveResult(string "name", image result_data)

saves result_data with an identifier “name” to the spreadsheet.

if result_data is vector, its coordinates (x, y), length and angle (measured anticlockwise from the horizontal axis) will be saved to the spreadsheet.

```
void PPAPrepArrow( string “name”, image vector_data, image start_point)
```

saves the vector_data and the start point to the spreadsheet for an arrow map.

```
void PPAPrepArrow( string “name”, image angle, image start_point)
```

saves the unit vector with the specified angle and the start point to the spreadsheet for an arrow map.

```
void PPAPrepColorMap( string “name”, image scalar_data, image display_point)
```

saves the scalar data and the display point to the spreadsheet for a color map.

Sample code

```
PPABeginDA()
```

```
// calculate the vector from an ideal position
```

```
image VirtualPeak := (PPAPeak(1)+PPAPeak(2)+PPAPeak(3)+PPAPeak(4))/4
```

```
// Here, we define the image “VirtualPeak” to which the center of the four peaks saved.
```

```
image displacement := PPAPeak(5) - VirtualPeak
```

```
PPASaveResult( “Ideal Position”, VirtualPeak )
```

```
PPASaveResult( “Displacement”, displacement )
```

```
PPAPrepArrow( “Displacement”, displacement, PPAPeak(5) )
```

```
//calculate angle between two vectors Peak(5) to Peak(2), and Peak(5) to Peak(1)
```

```
image angle := PPAngle( PPAPeak(5), PPAPeak(2), PPAPeak(1) )
```

```
PPASaveResult( “Angle”, angle )
```

```
PPAPrepColorMap( “Angle”, angle, PPAPeak(5) )
```

```
PPAFinishDA()
```

Another sample code

```
PPABeginDA()
```

```
// Here, we define the image “peakn” to which the coordinates of the peak #n is saved.
```

```
image peak1 := PPAPeak(1)
```

```
image peak2 := PPAPeak(2)
```

```
image peak3 := PPAPeak(3)
```

```
image peak4 := PPAPeak(4)
```

```
image peak5 := PPAPeak(5)
```

```
// calculate the vector from an ideal position
```

```
image VirtualPeak := (peak1+peak2+peak3+peak4)/4
```

```
// Here, we define the image “VirtualPeak” to which the center of the four peaks saved.
```

```
image displacement := peak5 - VirtualPeak
```

```
PPASaveResult( “Ideal Position”, VirtualPeak )
```

```
PPASaveResult( “Displacement”, displacement )
```

```
PPAPrepArrow( “Displacement”, displacement, peak5 )
```

```
//calculate angle between two vectors Peak(5) to Peak(2), and Peak(5) to Peak(1)
```

```
image angle := PPAngle( peak5, peak2, peak1 )
```

```
PPASaveResult( “Angle”, angle )
```

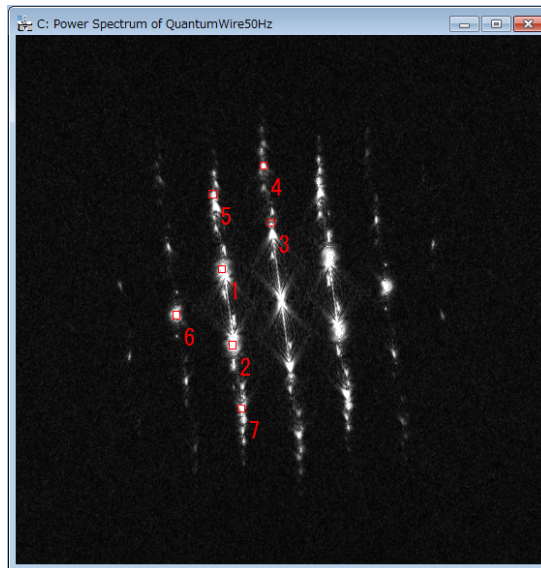
```
PPAPrepColorMap( “Angle”, angle, peak5 )
```

```
PPAFinishDA()
```

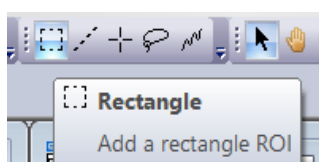
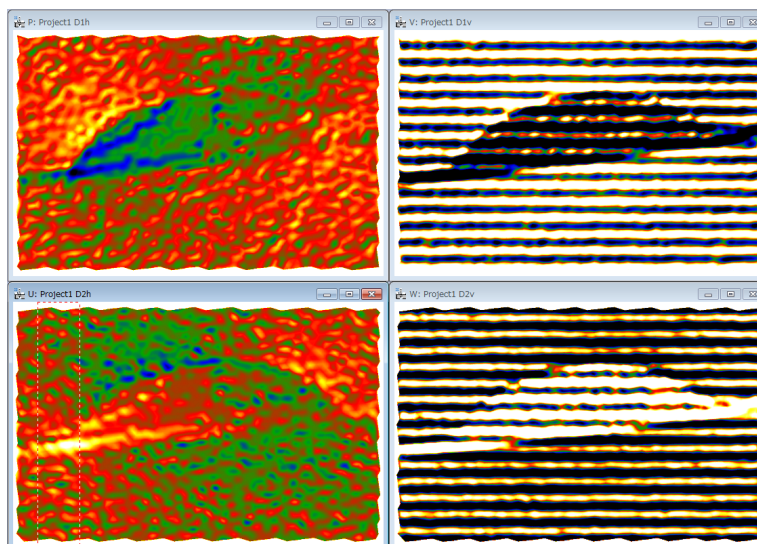

Correct scan line noise

There are situations in which the electron microscopy image is altered by the presence of scanning errors, such as small beam deflections due to external electromagnetic fields, as well as hysteresis effects during the ‘fly back’ between scan lines, that may severely distort strain results. The presence of scanning errors may be identified as the presence of annoying stripes in the strain results. In these cases, the option **Correct scan line noise** may be quite useful.

In order to show how to use this option, let us calculate strain results on the image QuantumWire50Hz.dm3 in the usual way, as we did with QuantumWire.dm3 image in previous pages. We will get the similar Power spectrum as shown below:

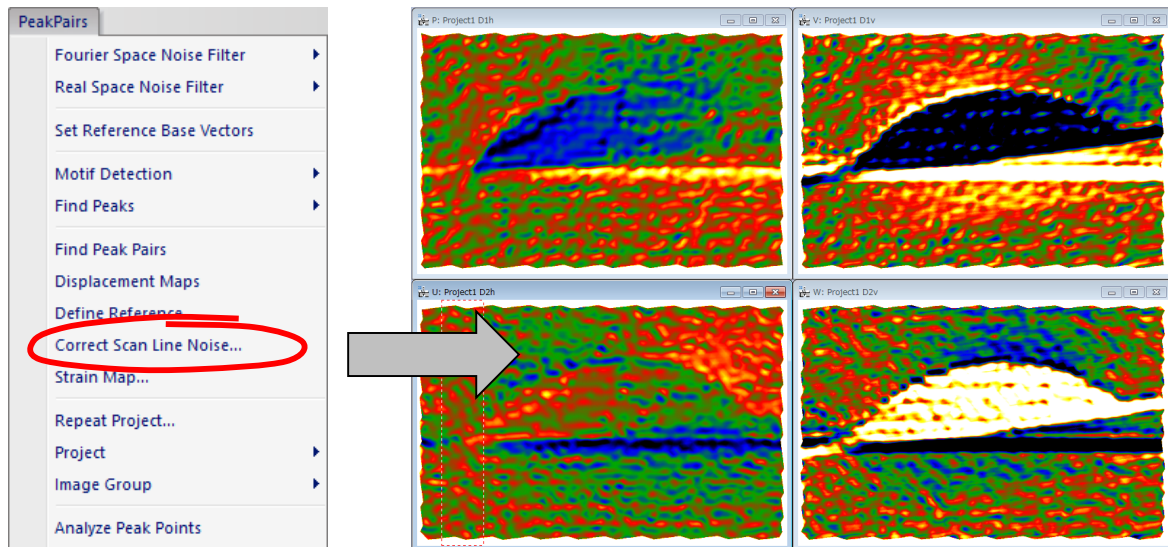


If we specify the lattice base vector (#1 and #2 as indicated), displacement maps shown below may be obtained. As we may observe, a set of stripes is shown in these maps:

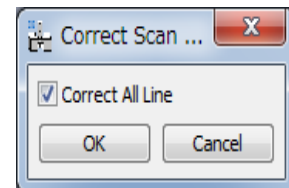


We can then Add a Rectangle ROI in one of the Displacement maps (here, the image U).

Then, press the **Correct Scan Line Noise** option to remove the stripes and determining a proper displacement map.

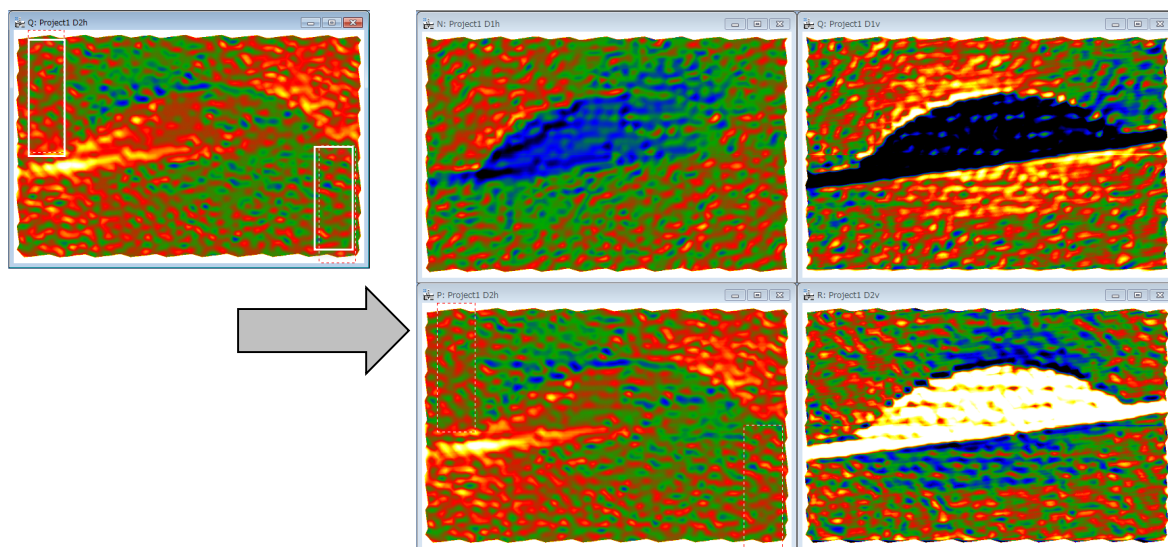


You can extend the reference area for the scan-line correction from the very top to the bottom lines, when you check “Correct All Line” in the dialog.



Unfortunately, in this example there is no perfect reference area from the top to bottom of this image. Therefore, we have horizontal artefacts as clearly see in the images V and W.

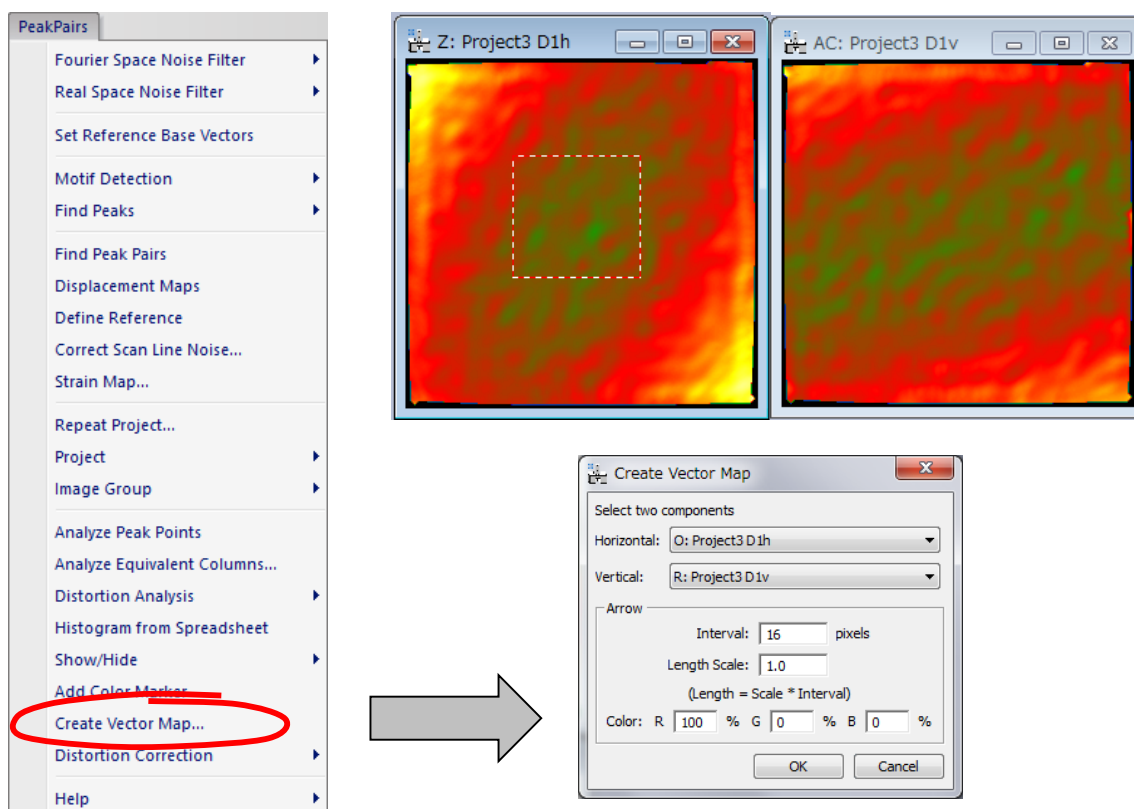
The scan-line correction has a capability to merge multiple reference areas. Here, we use two reference areas at the top left and the bottom right. Then, we can better perform the scan-line distortion as shown below. There is no appreciable artefact observed before.



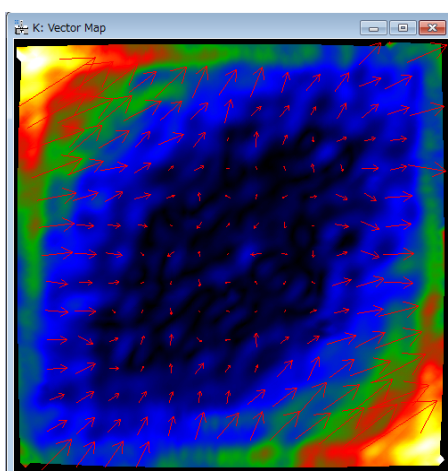
Create Vector maps

It is possible to create a vector map from *two vector components*, such as D1h and D1v. To do so, launch the **Create Vector Maps** command, and select two vector component images of the associated vector map.

We explain here this function using the displacement maps, D1h and D1v, calculated from *Substrate.dm3*. After launching the **Create Vector Map** command, select these two images, D1h and D1v, and press OK.



Then, you will get a colour map corresponding to the vector magnitude, with arrows showing the directions and magnitudes of the vectors as shown below:

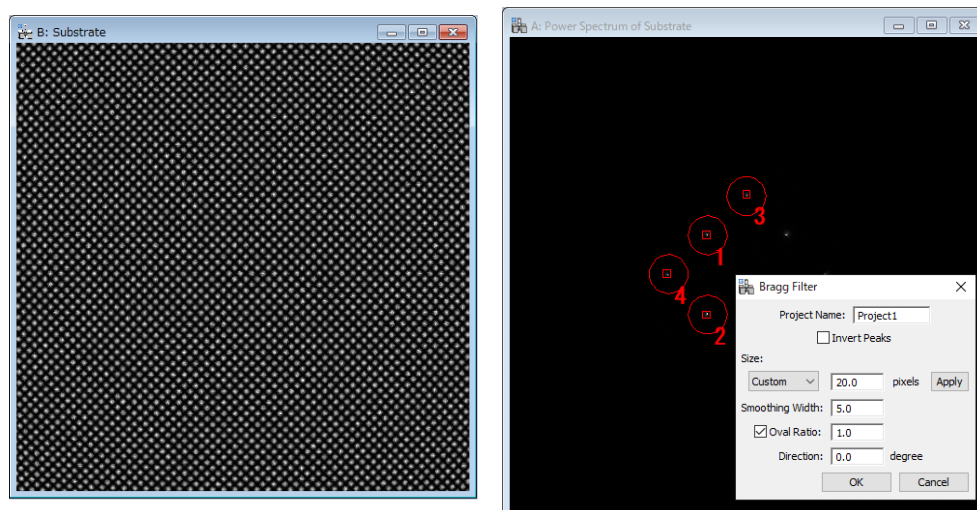


The vector map here is a complex DM image, whose real and imaginary parts correspond respectively to the Horizontal and Vertical images selected in the dialog.

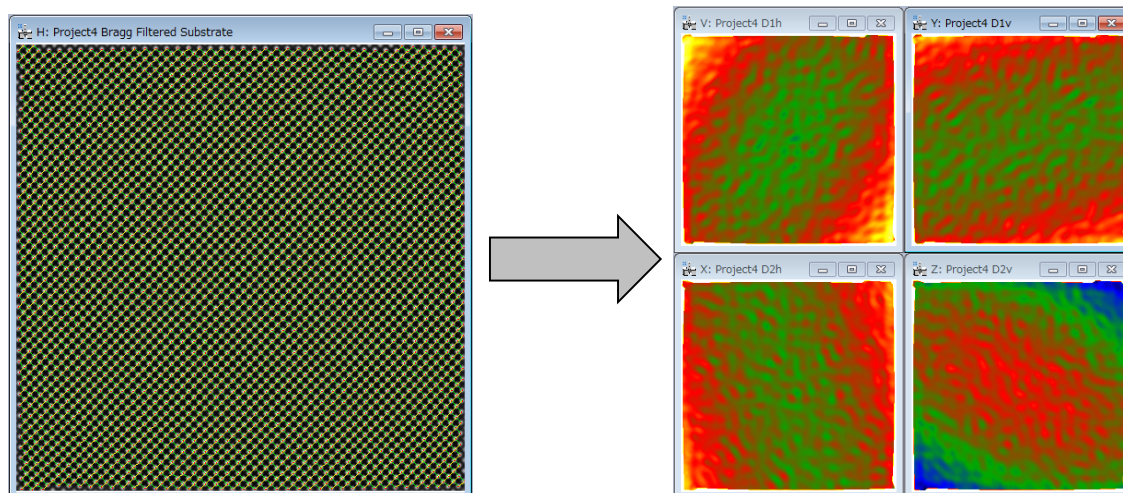
Image rectification

This command allows the user to correct any distortion from an image of a perfect crystal, using Peak Pairs information. We explain here distortion correction using an image corresponding to a perfect crystal, *Substrate.dm3*.

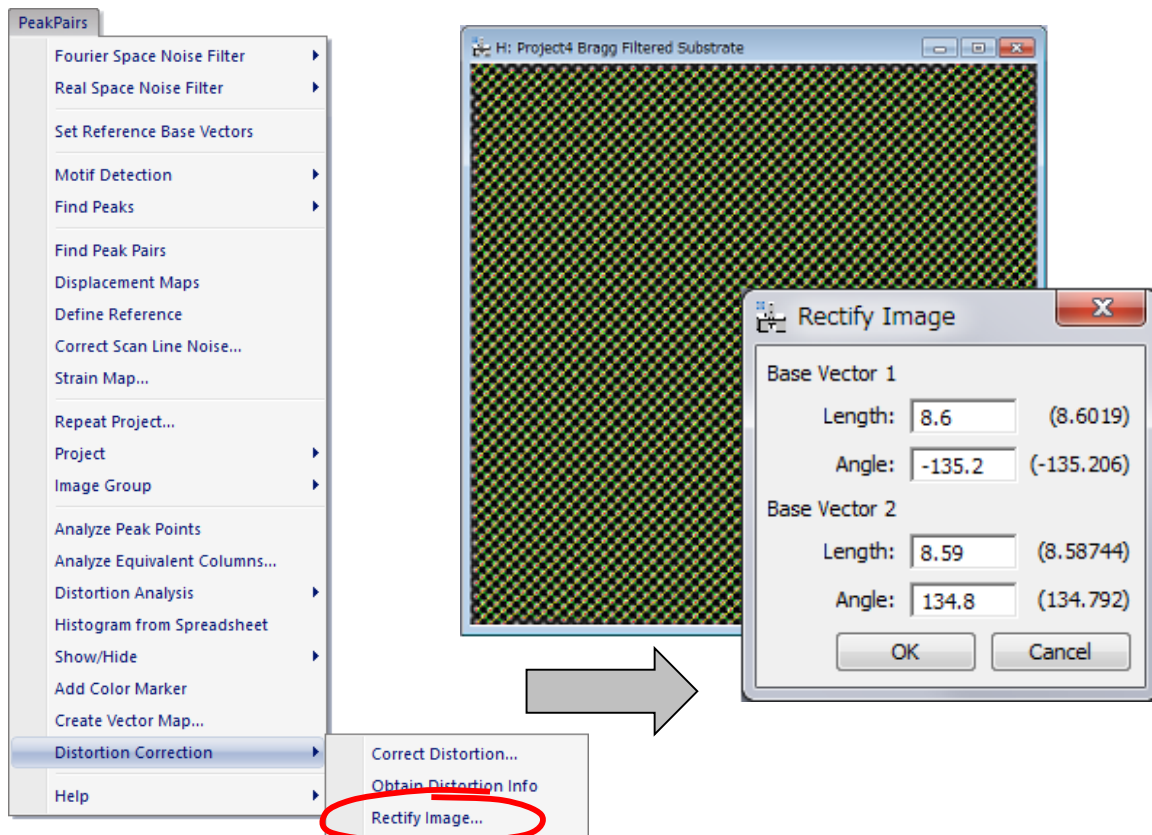
Open the image *Substrate.dm3*, execute the **Power Spectrum**, and then **Bragg Filter** in the usual way by selecting relevant spots in the Power Spectrum.



Then calculate the *Peak Pairs* using the usual commands (**Find Peaks** followed by **Find Peak Pairs**). If we analyse the displacements with the **Displacement Maps** command, we can observe that the image of a perfect crystal is distorted as shown below.

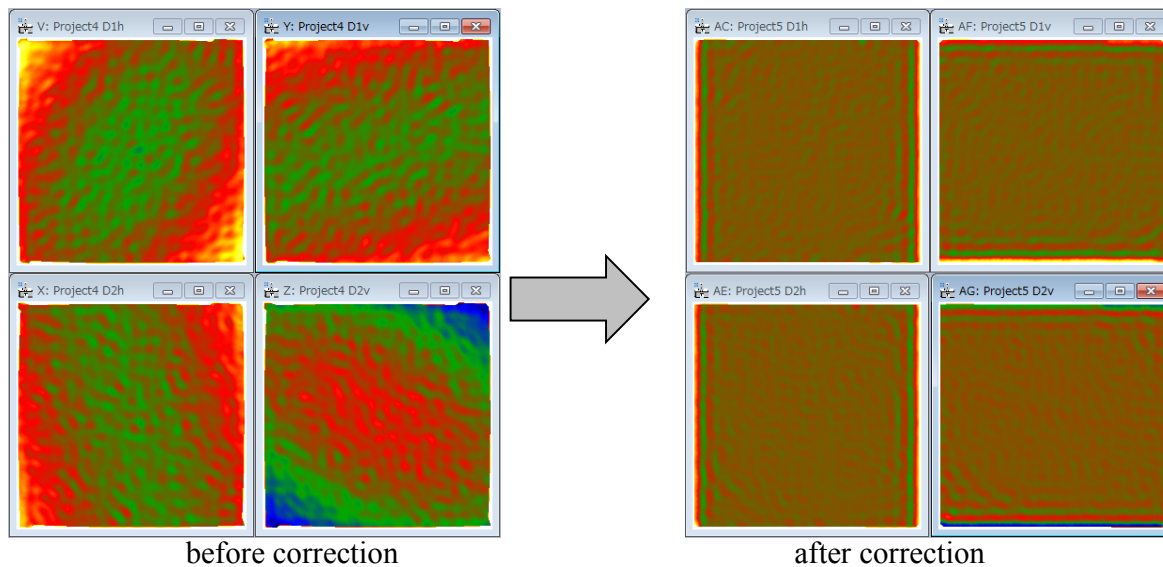


Given that the image corresponds to a perfect crystal, we can get a rectified image. In order to do that, select the project image with Peak Pairs information, and then apply the **Rectify image** command.



The lengths and angles of current reference base vectors will be shown in the dialog. If the values in the parentheses differ from the values expected from an ideal unit cell, you can change the values accordingly.

By pressing OK, the distorted image is rectified using the local distortions at each point of the image. To verify this, calculate the displacement maps from the rectified image. Then, we observe that distortions have been corrected as shown below:



Appendix

Technical Note:

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 :

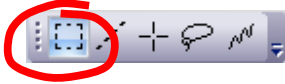
$$\Delta_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_i} + \frac{\partial u_j}{\partial x_j} \right) \text{ i.e. } \Delta_{xy} = \frac{1}{2} (\varepsilon_{xx} + \varepsilon_{yy})$$

Rotation (in radians and anti-clockwise positive):

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

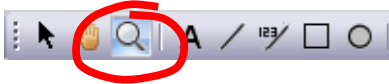
Some useful DM tricks

DM ROI tool:



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

DM Zoom tool:



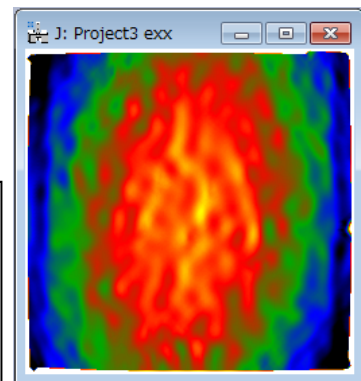
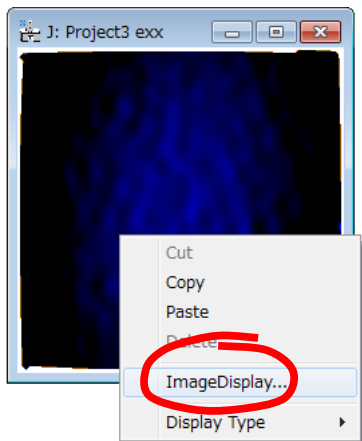
Hint: to demagnify, press ALT.

HREM Mouse tool



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

DM Image Display Command

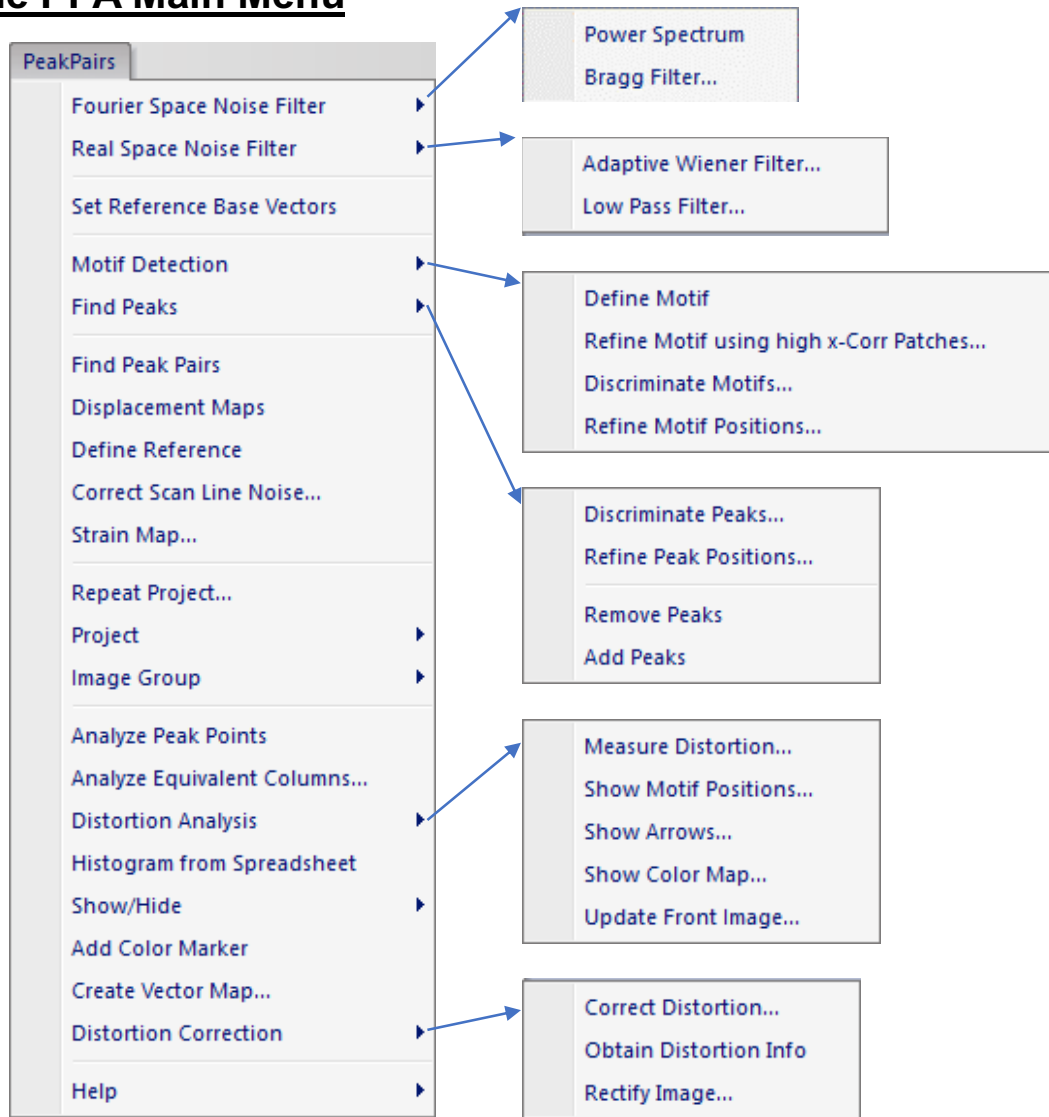


Hint: to change the color map of any image, press the right mouse button on it, select ImageDisplay, and modify the options as desired.

For example, it is useful to set manually the color range of each map to be the same, so as to be able to compare each other.

Quick Reference Guide

The PPA Main Menu



The commands in the PPA menu are described below.

| Command | Description |
|--|--|
| Fourier Space Noise Filter (see sub menus) | Reduces noise using Fourier space filter. |
| Real Space Noise Filter (see sub menus) | Reduces noise using Real Space Filter. |
| Set Reference Base Vectors (see Dialog) | Set the reference base vectors manually on a real-space noise-filtered image or an image after Motif detection. Note: Bragg filter sets the reference base vectors automatically. |
| Motif Detection (see sub menus) | Detects repeating units (a group of peaks) using a Motif (small reference region). |
| Find Peaks (see sub menus) | Locates peaks of intensity in an image. Note: Reference base vectors should be defined beforehand. |
| Find Peak Pairs | Calculates pairs of peaks along two reference base vectors automatically. |
| Displacement Maps | Generates horizontal and vertical displacements along the two directions defined by the basis vectors |
| Define Reference | Changes the displacement values, so as to obtain a uniform displacement in the chosen area. Note: the area should be selected previously using the ROI tool on any displacement image |
| Correct Scan Line Noise... | Corrects imperfect scan-line control (scan-line noise) of the STEM scanning system using a perfect area in the image. Note: the area should be selected previously using the ROI tool on any displacement image. |
| Strain Map... (see Dialog) | Calculates strain maps (e_{xx} , e_{yy} , e_{xy} and e_{yx}) at any desired angle. |
| Repeat Project... (see Dialog) | Generates strain maps and other outputs for the front most image using the same conditions of a selected project. |
| Project (see sub menus) | Menu to manage all the images in a particular project. |
| Image Group (see sub menus) | Menu to close or save groups of images within a particular project. |
| Analyze Peak Points | Generates a spreadsheet of data (peak position, peak intensities, strain values) for each peak |
| Analyze Equivalent Columns... (see Dialog) | Analyzes equivalent column positions, as well as the distances and angles between specified columns. The independent column(s) will be specified using the HREM Mouse tool. |

| | |
|---|---|
| Distortion Analysis (see sub menus) (from v4.0) | Analyzes peak distances or angles of the peak-pairs, or rotation angles of structural units (e.g. tetrahedron or octahedron). The advanced analysis can be performed using the DM script that simply calls the functions provided by the PPA. |
| Histogram from Spreadsheet | Calculates a different histogram for each selected column in the spreadsheet |
| Show/Hide (see sub menus) | Shows/hides a selected annotation on the image. |
| 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.) |
| Create Vector Map... (see Dialog) | Create a vector map from two component images selected in the dialog. |
| Distortion Correction (see sub menus) | Eliminates systematic distortions present in the image based on the measurement of an ideal distortion-free image. |

Fourier Space Noise Filter SubMenu

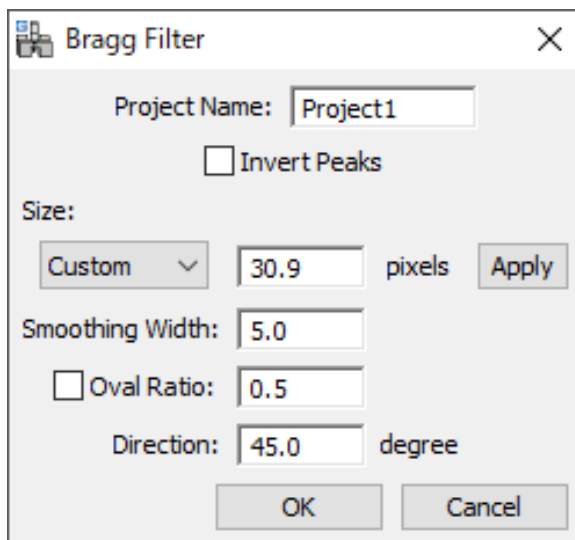


| Component | Description |
|---------------------------------|---|
| Power Spectrum | Calculates the Fourier transform of the front most image, and displays the power at each frequency (commonly called the Power Spectrum). |
| Bragg Filter... (see Dialog) | Calculates Bragg Filter using the spots selected in the Power Spectrum. The shape and size of the mask can be defined by the user in the dialog. Note: Spots should be selected beforehand in the Power Spectrum using the Mouse Tool. Note: The first and second spots defined the Reference Base Vectors in real space. |

Bragg Filter Dialog

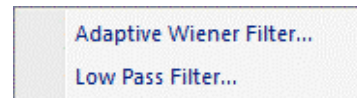
The components of the dialog are described below.

Dialog



| Component | Description |
|-----------------|---|
| Project Name | Name given to the group of images and results |
| Invert Peaks | If you want to analyze the hollows (dips), not peaks, you should check this item. |
| Size | Defines mask radius of hard cut-off (beyond which values are set to zero). |
| Smoothing Width | Specifies mask smoothing width in pixels |
| Oval Ratio | Defines the shape of the oval, as major to minor axis ratio |
| Direction | Sets the prescribed masks angle, in degrees |

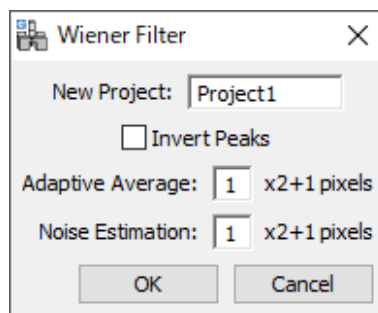
Real Space Noise Filter SubMenu



| Component | Description |
|---|--|
| Adaptive Wiener Filter... (see Dialog) | Remove noise from the image using an adaptive Wiener filter based on a local variance. |
| Low Pass Filter... (see Dialog) | Calculates and applies a Low Pass filter to the image |

Adaptive Wiener Filter Dialog

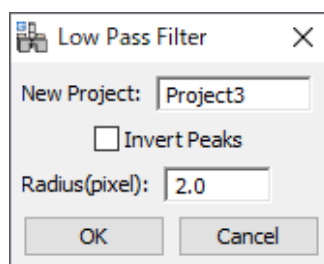
Dialog



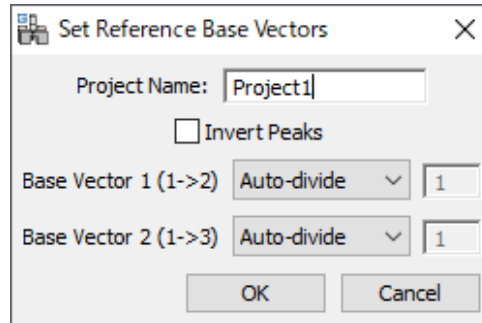
| Component | Description |
|------------------|--|
| New Project | Name given to the group of images and results |
| Invert Peaks | If you want to analyze the hollows (dips), not peaks, you should check this item. |
| Adaptive Average | Window size [(2N+1)x(2N+1) pixels] to be used in the calculation of the adaptive average |
| Noise Estimation | Window size [(2N+1)x(2N+1) pixels] to be used in the calculation of the noise estimation |

Low Pass Filter Dialog

Dialog



| Component | Description |
|---------------|---|
| New Project | Name given to the group of images and results |
| Invert Peaks | If you want to analyze the hollows (dips), not peaks, you should check this item. |
| Radius(pixel) | The radius of the mask in pixels |

Set Reference Base Vectors Dialog**Dialog**

| Component | Description |
|---------------------|--|
| Project Name | Name given to the group of images and results |
| Invert Peaks | If you want to analyze the hollows (dips), not peaks, you should check this item. |
| Base Vector 1 and 2 | You can select Auto-divide or specify the number of repeating units along two directions. |

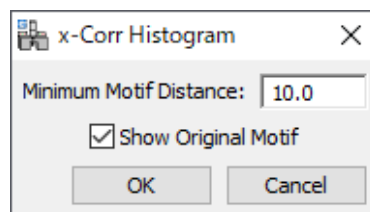
Motif Detection SubMenu



| Component | Description |
|--|---|
| Define Motif | Defines a Rectangle ROI as a Motif, and make it rotatable. |
| Refine Motif using high x-Corr Patches... (see Dialog) | Calculates Cross-Correlation Histogram between the selected reference region (motif) and the original image, and refines the motif using high-scored pathes. Note: The left edge of the selection in the histogram is used as a threshold to obtain the refined motif. |
| Discriminate Motifs | Calculates Cross-Correlation Histogram between the refined motif and the original image, and refine again the motif using high-scored pathes. Note: The left edge of the selection in the histogram is used as a threshold to find good motifs. |
| Refine Motif Positions... (see Dialog) | Refines the centers of good Motifs in the image. |

Refine Motif using high x-Corr Patches Dialog

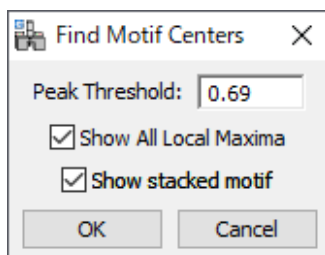
Dialog



| Component | Description |
|------------------------|--|
| Minimum Motif Distance | Specifies a minimum distance between allowed motifs. (This parameter is used in Find Motif Centers...) |
| Show Original Motif | If checked, the original motif will be displayed. |

Refine Motif Positions Dialog

Dialog



| Component | Description |
|-----------------------|--|
| Peak Threshold | Specifies a minimum for the intensity of allowed Peaks. |
| Show All Local Maxima | If checked, the Motif centers rejected by the cross-correlation threshold and/or the motif distance will be shown in blue. (Namely, all the motif centers are displayed in red or blue color.) |
| Show stacked motif | If checked, a stacked image from detected motifs will be created. |

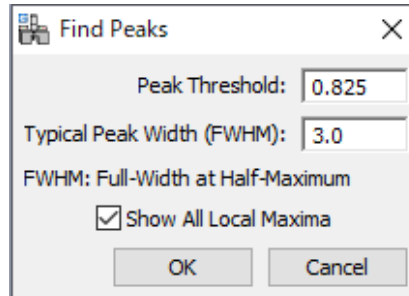
Find Peaks SubMenu



| Component | Description |
|--|---|
| Discriminate Peaks | Calculates a histogram of peaks intensities, helping the user to determine a precise value for Peak Threshold. Note: The left edge of the selection in the histogram is used as a threshold to find good peaks. |
| Refine Peak Positions... (see Dialog) | Refines peak positions by fitting a quadratic function to peak intensity, and then calculates a histogram of the peak heights of the quadratic function. The peaks within a minimum distance will be merged. Note: The left edge of the selection in the histogram is used as a threshold to find good peaks. |
| Remove Peaks | Remove the peaks, which are selected by using HREM Mouse . |
| Add Peaks | Refine and add the peaks, which are selected by using HREM Mouse . |

Refine Peak Positions Dialog

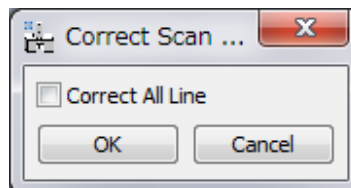
Dialog



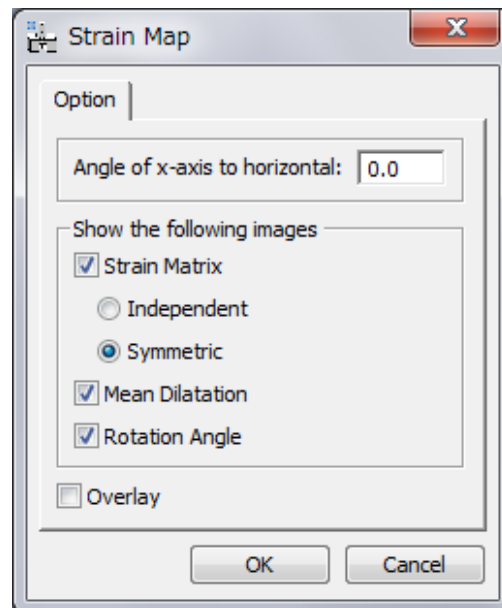
| Component | Description |
|---------------------------|--|
| Peak Threshold | Specifies a minimum for the intensity of allowed peaks |
| Typical Peak Width (FWHM) | Specifies a typical peak width (FWHM in pixels). This value will be used to merge the peaks. |
| Show All Local Maxima | Shows local maxima (of 8-neighbourhood) as blue points. |

Correct Scan Line Noise Dialog

Dialog



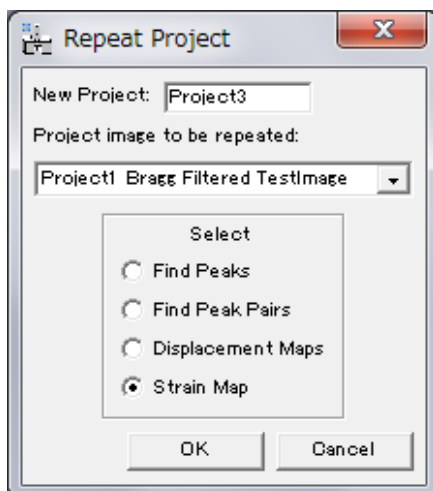
| Component | Description |
|------------------|--|
| Correct All Line | It modifies all scan lines, not only those within the ROI. |

Strain Map Dialog**Dialog**

| Option | Description |
|-------------------------------|--|
| Angle of x-axis to horizontal | Specifies the angle of the direction to be considered as x-axis. You can specify the orientation of the x-axis by placing a Line ROI on the HREM image. In this case, the angle of the Line ROI appears here automatically. Note: If angle is set equal to 0, horizontal and vertical directions are assumed to be x and y coordinate axis respectively. |
| Strain Matrix | Specifies the images to be shown |
| Independent | Images of du/dx , du/dy , dv/dx , dv/dy to be displayed |
| Symmetric | 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. |
| Overlay | Shows the strain at each atomic column, and displayed as coloured dots over the original image |

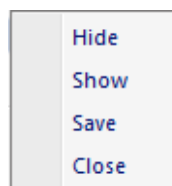
Repeat Project Dialog

Dialog



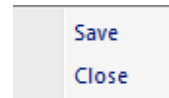
| Component | Description |
|------------------------------|---|
| New Project | Defines the name of the new project. |
| Project image to be repeated | Selects an open project to be used to generate strain maps and other outputs for the front most HREM image. Note: If you want to use the project created during the previous session, you may want to open it again. |
| Find Peaks | Repeats Find Peaks Operation. |
| Find Peak Pairs | Repeats Find Peak Pairs Operation. |
| Displacement Maps | Repeats Displacement Maps Operation. |
| Strain Map | Repeats Strain Map Operation. |

Project Sub-Menu



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

Image Group Sub-Menu

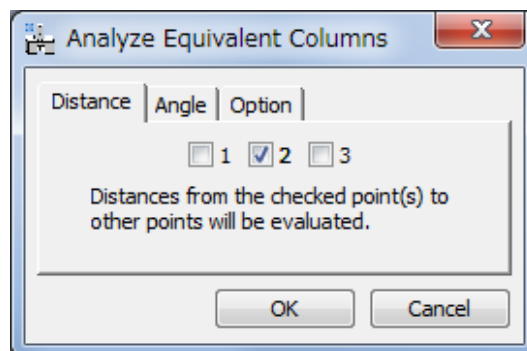


| Component | Description |
|-----------|--|
| Save | Saves (with dialog) all images in a project of the same type as the front most image (e.g. strain map images). |
| Close | Closes (without saving) all images of the same type as the front most image. |

Analyze Equivalent Columns Dialog

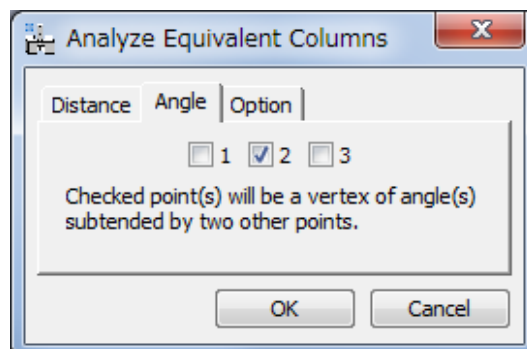
The user will have the option to decide the distances and/or angles to be evaluated.

Distance Tab



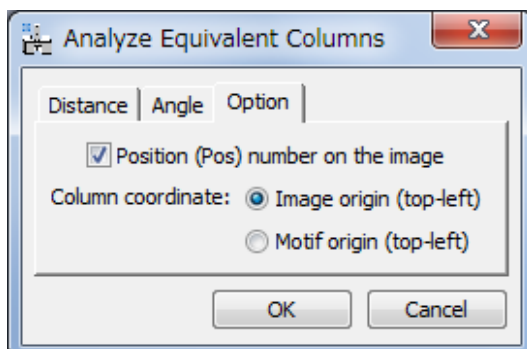
The number of each check box corresponds to the assigned number to the mouse click. All the distance(s) from the checked point to other points will be calculated.

Angle Tab



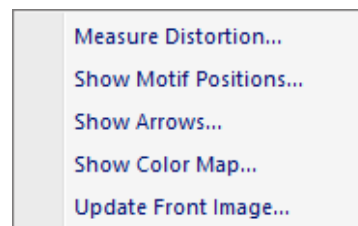
The number of each check box corresponds to the assigned number to the mouse click. All possible angle(s) whose vertex corresponds to the checked point will be calculated.

Option Tab



| Component | Description |
|------------------------------------|---|
| Position (Pos) number on the image | Display position number (Left column of the spread sheet) on original image. |
| Column coordinate | (Motif Detection only) You can select the origin of column positions in the Motif. |

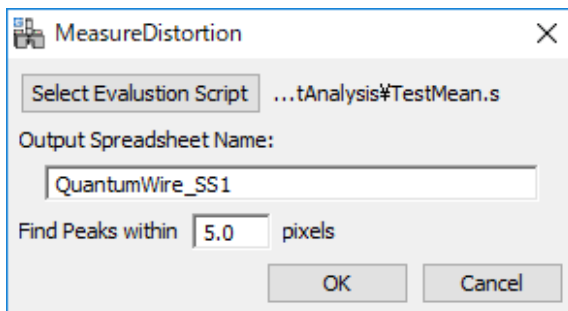
Distortion AnalysisSub-Menu
(from v4.0)



| Command | Description |
|-------------------------|---|
| Measure Distortion... | At first, distortion values will be measured by running the saved script. This command will open the dialog to select the script. NOTE: Alternatively, the distortions will be directly measured by executing the script from the script window. |
| Show Motif Positions... | Displays the evaluated motif positions. |
| Show Arrows... | Displays the distortions measured by using <i>PPAPrepArrow</i> in an arrow map. |
| Show Color Map... | Displays the distortions measured by using <i>PPAPrepColorMap</i> in a color map. |
| Update Front Image... | Updates the appearance of the arrow or color map according to the modified appearance parameter(s). The dialog for the arrow map or color map will be opened according to the type of the front image. |

Measure Distortion Dialog

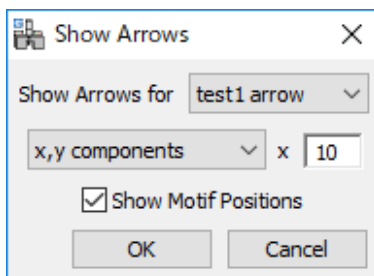
Dialog



| Component | Description |
|--------------------------|--|
| Select Evaluation Script | Clicking on this button will open the file browser to select the saved script. NOTE: If you directly execute the script from the script window, you will have a dialog without the file selection capability. |
| Output Spreadsheet Name | Specify an output spreadsheet name. The measured distortion values will be saved as a spreadsheet. |
| Find Peaks within | Peaks will be searched in the specified area in pixel from the corresponding points in the Motif. |

Show Arrows Dialog

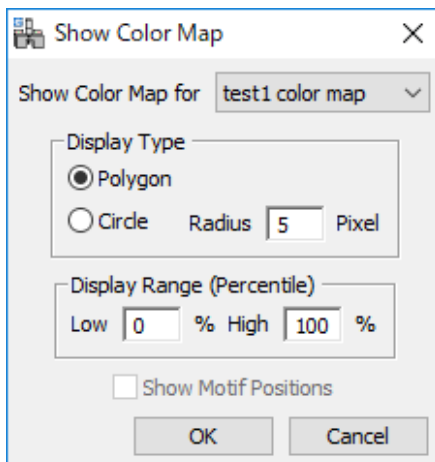
Dialog



| Component | Description |
|-----------------------|---|
| Show Arrows for | Select the column in the spreadsheet corresponding to the measured values to draw an arrow map. |
| Output value selector | Select the value(s) to draw an arrow. |
| Show Motif Positions | Shows the potions of the approximate motif centers. |

Show Color Map Dialog

Dialog

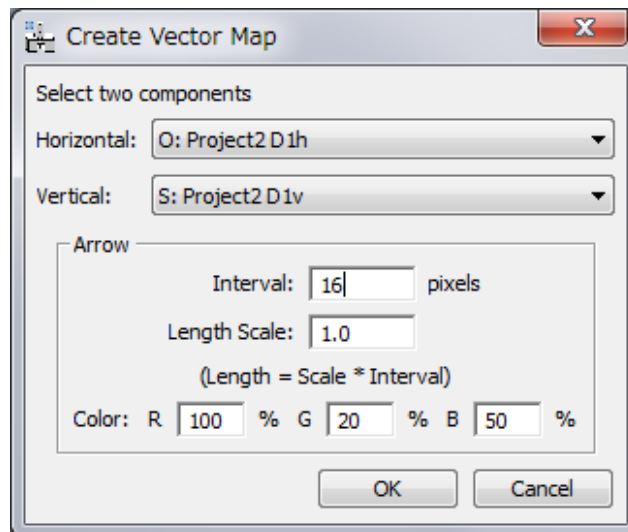


| Component | Description |
|----------------------|--|
| Show Color map for | Select the column in the spreadsheet corresponding to the measured values to draw a color map. |
| Display Type | Select the display type from Polygon and Circle. In the case of the circle, the radius of the circle can be specified. |
| Display Range | The display ranges will be specified in percentiles. |
| Show Motif Positions | If the display type is Circle, the positions of the approximate motif centers can be drawn. |

Show/Hide Sub-Menu



| Command | Description |
|------------|---|
| Peaks | Displays the circle at the peak positions on the image. |
| Peak Pairs | Displays the peak-pair lines on the image. |
| Motif | Shows/hides Motif |

Create Vector Map Dialog**Dialog**

| Component | Description |
|------------------|--|
| Horizontal | Select an image corresponding to the horizontal component. |
| Vertical | Select an image corresponding to the vertical component. |
| Interval | Specifies an interval to draw arrows (in pixel) |
| Length Scale | Specifies an arrow length. An actual length is Interval * Scale (in pixel) |
| Color | Specifies an arrow color in RGB. |

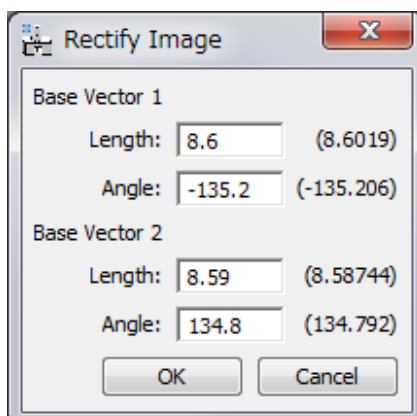
Distortion Correction Sub-Menu

Correct Distortion...
Obtain Distortion Info
Rectify Image...

| Command | Description |
|----------------------------------|--|
| Correct Distortion... | Rectifies any distorted image using the distortion information obtained previously from an undistorted sample using the "Obtain Distortion Info" command below. A dialog to select two images will be opened. |
| Obtain Distortion Info | Extracts distortion information from the Bragg image of an undistorted crystal after calculating Peak Pairs. This information will be used by the "Correct Distortion" command above. |
| Rectify Image... (see Dialog) | Rectifies an image of an undistorted crystal after calculating Peak Pairs. Default basis vector are automatically chosen from the first and second selected Bragg spots. Basis vectors can also be manually specified/modified by the user. |

Rectify Image Dialog

Dialog



| Component | Description |
|------------------|--|
| Length | Length of base vector considered for image rectification, measured in pixels |
| Angle | Angle of base vector considered for image rectification, measured in degrees |