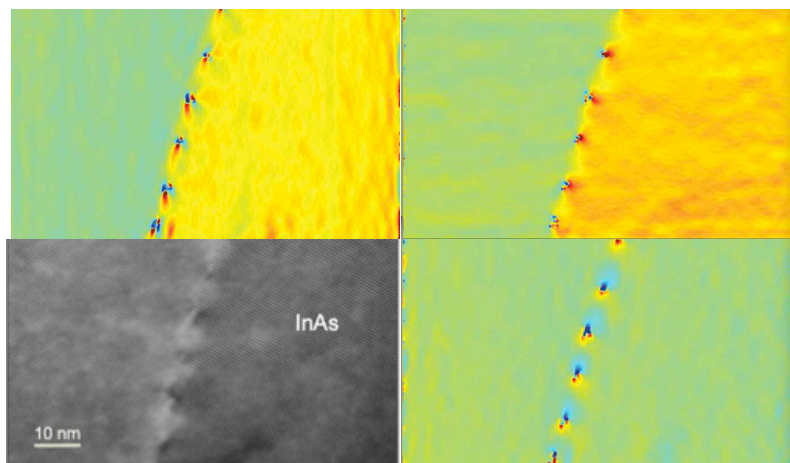# *PPA for DigitalMicrograph*

Peak Pairs Analysis

*High-Resolution Peak Measurement
and Strain Mapping Analysis*

InAs

10 nm

PPA User Manual v3.5

HREM Research Inc.

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Acknowledgements

The scientific developer of this method (Prof. Pedro L. Galindo) would like to acknowledge to all authors of the references cited in this manual for their collaboration in the process of its application to the scientific problems presented in these cited papers.

Copyright Statements

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.
Italics	Used to denote emphasis, captions and the result of an action in a procedure.

Table of contents

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^{TM})
- 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.
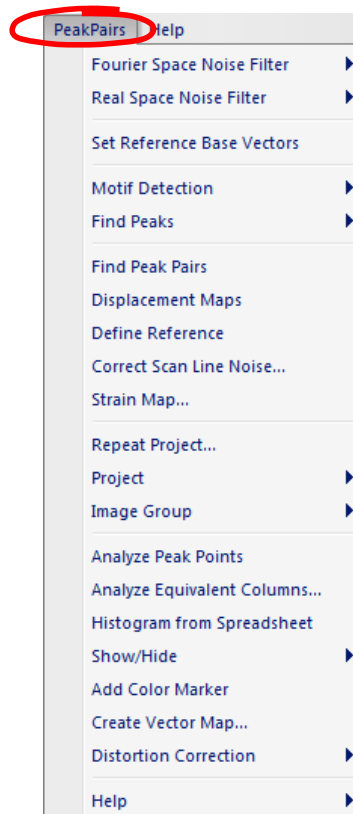
Installing IPU Plug-in
The PPA plug-in uses some functions based on the Intel' MKL (Math Kernel Library) provided by the IPU plug-in. All the files relating the IPU plug-in can be installed by copy-and-paste copy. The IPU plug-in will appear as under *IPU* menu. Please consult the ReadMe file that comes 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.

PeakPairs Help
Fourier Space Noise Filter ▶
Real Space Noise Filter ▶
Set Reference Base Vectors
Motif Detection ▶
Find Peaks ▶
Find Peak Pairs
Displacement Maps
Define Reference
Correct Scan Line Noise...
Strain Map...
Repeat Project...
Project ▶
Image Group ▶
Analyze Peak Points
Analyze Equivalent Columns...
Histogram from Spreadsheet
Show/Hide ▶
Add Color Marker
Create Vector Map...
Distortion Correction ▶
Help ▶

# *Getting Started*

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

Open the file *QuantumWire.dm3* using the DM command File…Open:
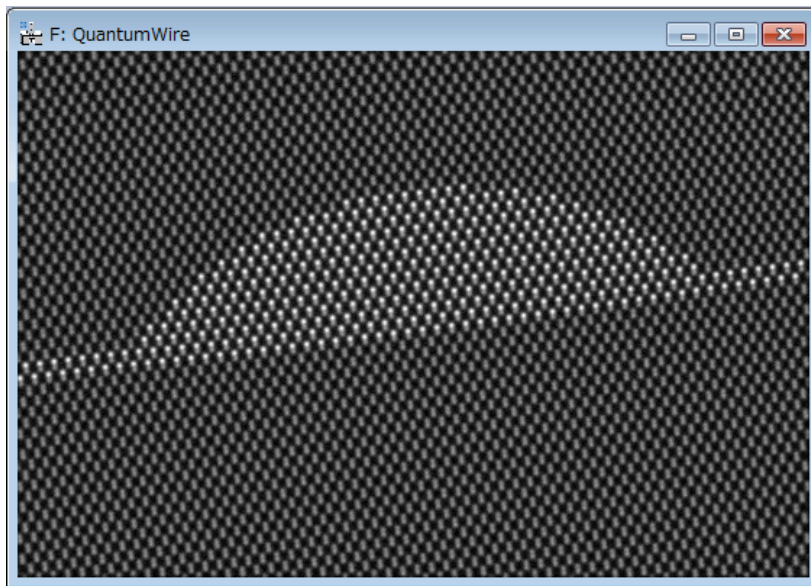
This image represents a capped InAs quantum wire on GaAs.

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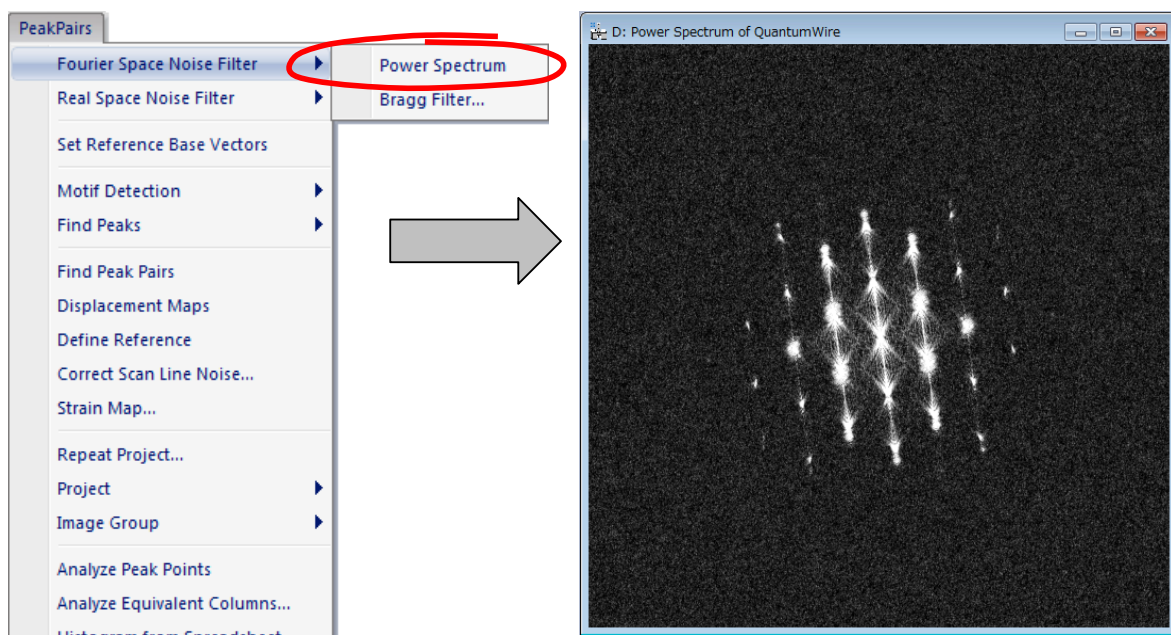
Now, select the **HREM mouse** tool**,** and click on desired spots to apply Bragg filter. The usual choice is to select the brightest spots in the spectrum, but those corresponding to higher harmonics can also be selected:

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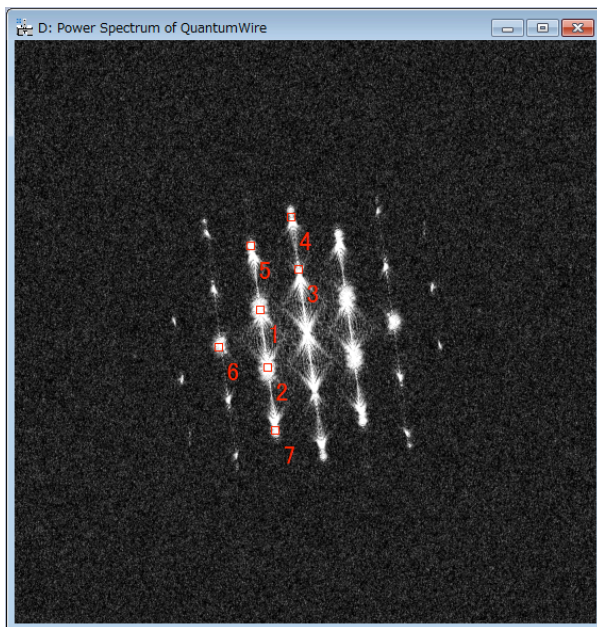
> **Hint:** if you wish to delete any spot, just click on the mouse mark again with the SHIFT key down.

> **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.
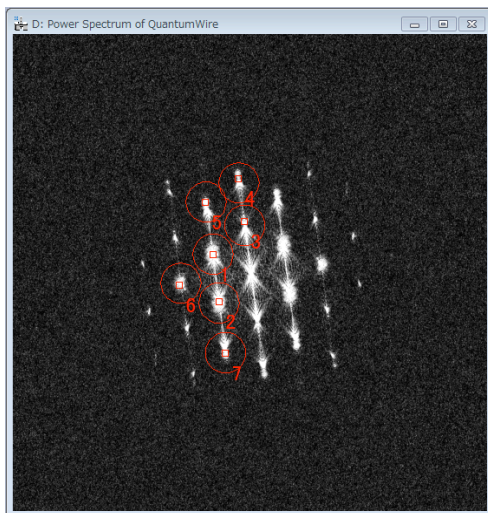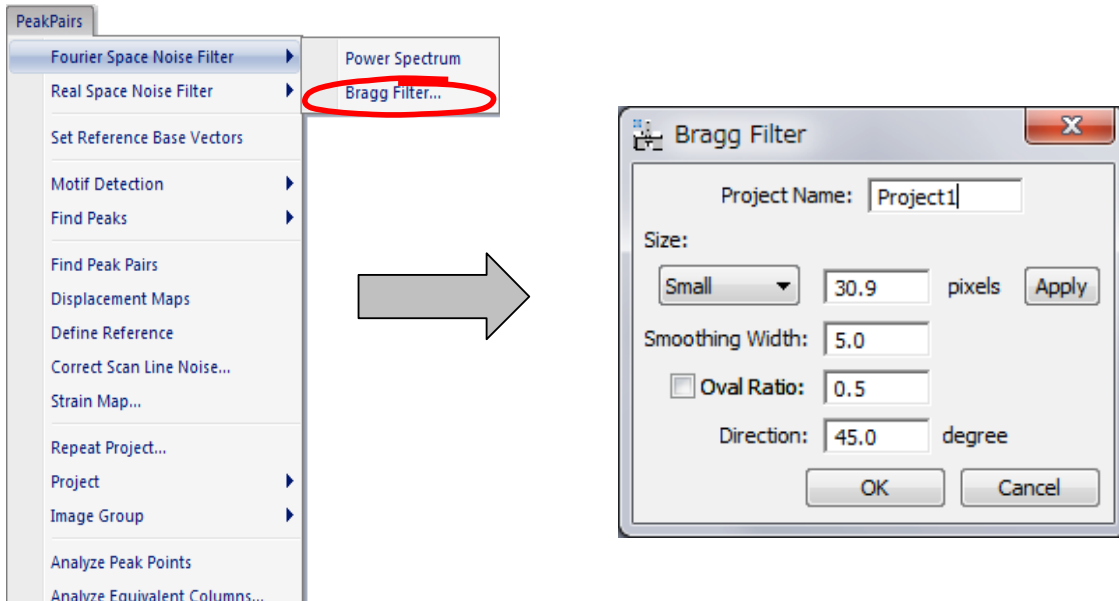

The shape and size of the Bragg filter must be adjusted such that no loss of information occurs. In this dialog box we can determine the size (in pixels), smoothing width(in pixels), oval ratio(height/width) and direction(in degrees) of mask spots.

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.
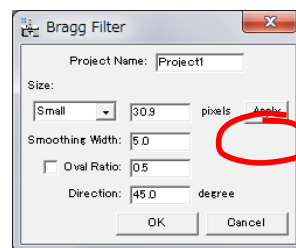
Let us select the first option (small window, oval ratio=1) and press the OK button, and the Bragg filtered image will appear immediately.

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.
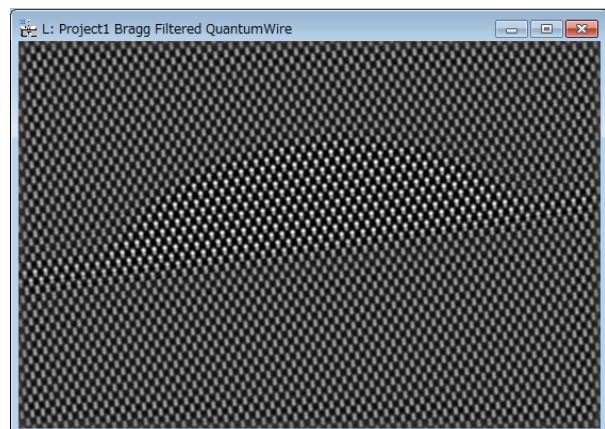
Peak Detection (for simple structure images)

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 approach to peak detection is based on peak identification based on their intensities.

The **Peak Histogram** command detects all intensity maxima in the image, and calculates the histogram of peak intensities.

The histogram allows the user locating different sets of peaks, based on their intensities, for determining strain. This discrimination is obtained by defining a lower threshold using the histogram. All peaks of intensity lower than this threshold are discarded.
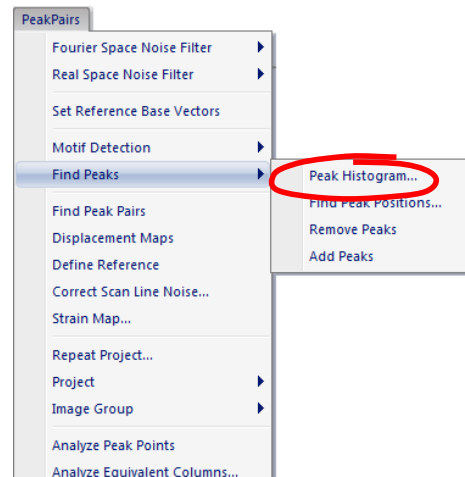
Here, we use *Test image.dm3* as a sample data. First, we apply the Bragg filter using all the spots in the Power Spectrum. When the command **Peak Histogram** is issued, the following dialog box allows the user to specify if the user is interested in white (unchecked) or black spots (checked) using the Invert Peaks checkbox option
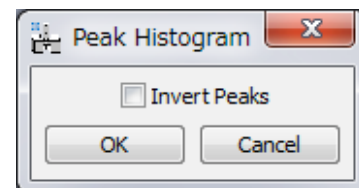
After clicking OK, the HREM Histogram tool shown right will appear as well as a new window showing the histogram of all the peaks found in the image. The default range of the histogram is set to the maximum and minimum of the peaks. If you want, you can change the histogram range as well as the number of bins. When you change these values, push the "Apply" button.
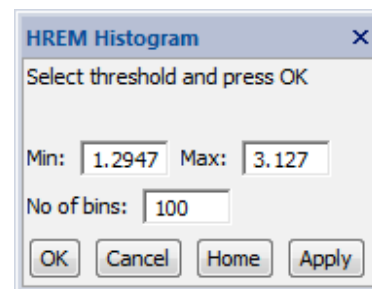
Once the histogram is shown, the user should select the intensity threshold for identifying which peaks will be used in further analysis. To do so, just click the mouse on the histogram, and select the desired range of peaks. The left side of the selection made in the histogram will be used in the following **Find Peak Positions** command.
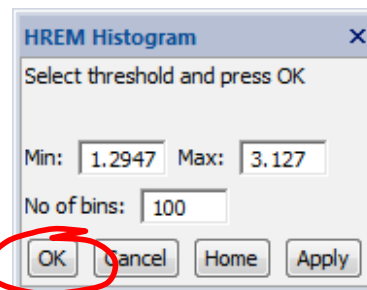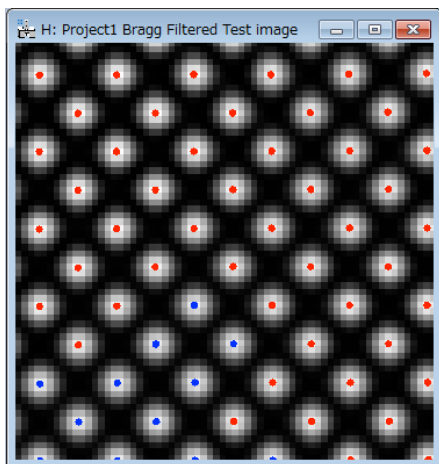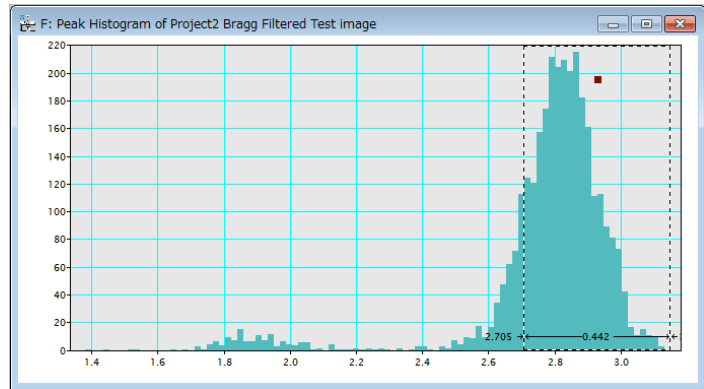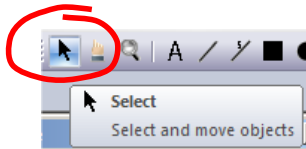
The discovered peaks will be classified to red or blue depending on the peak values: red indicate the peak that is higher value than the selected threshold, while blue indicate the peak equal to or lower than the threshold. The peak colour will be dynamically revised by changing the threshold (the left-edge 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 **Find Peak Positions**.
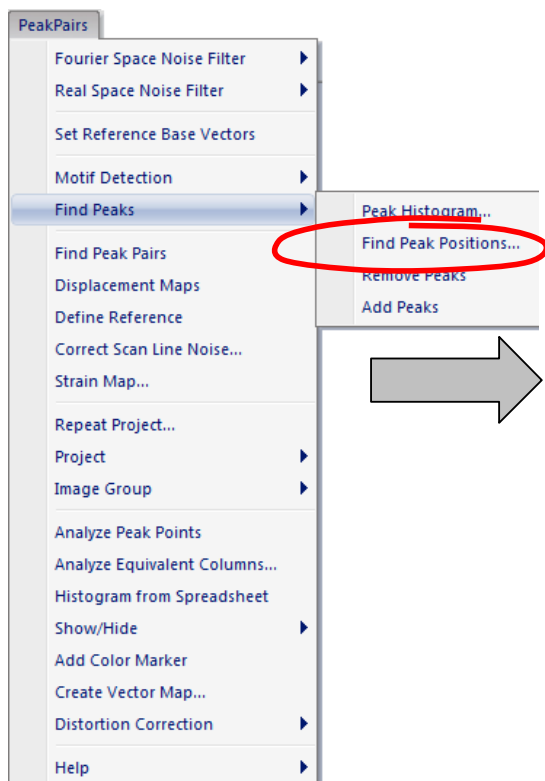

The following dialog box appears:
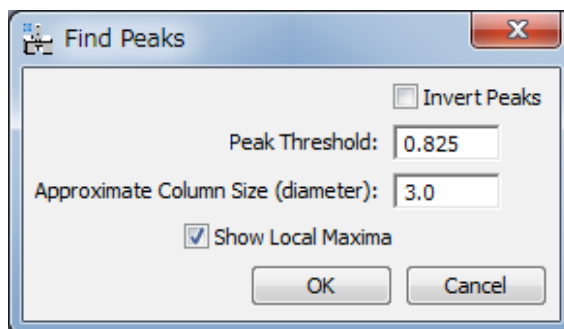
Peak Threshold indicates the minimum intensity of a point to be considered as a valid peak. Peaks having intensities below this threshold will be discarded. Peak threshold value is automatically read from the left side of the selection made in the histogram. However, the user can manually modify this value, if necessary.

You may want to use Approximate Column Size (in pixel) to merge the peaks (columns) within the specified column size.

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 analytically the maxima, as described in the reference for the algorithm in the Introduction section.
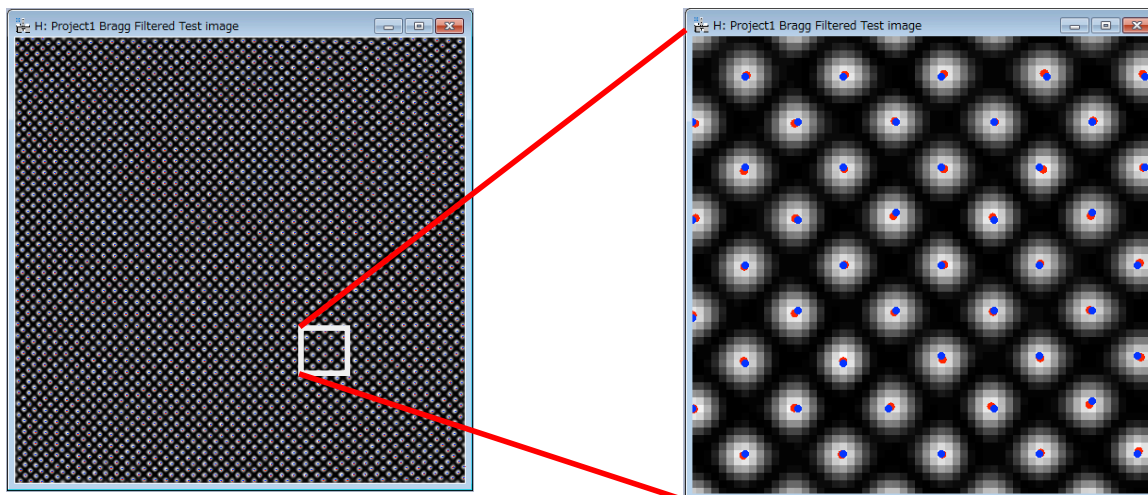

Sometimes, extra peaks are obtained in this automatic Peak Finding process, especially at the borders of the image. Repeating the **Find Peaks** command with a new Peak Threshold, all peaks in the border of the image will be discarded and won't be considered in any further calculations.

Motif Detection (for complex structure images)

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.
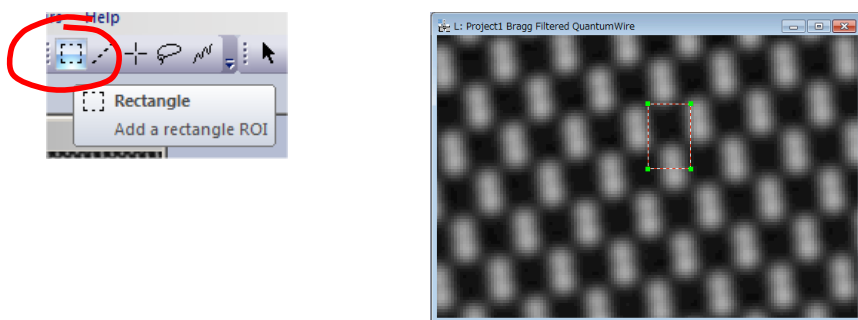
Once the rectangle ROI has been placed, you can rotate the Motif ROI, if you want. To do so, please select the **Define motif** in the Motif Detection submenu. (how to rotate the ROI, consult the Define Reference command)
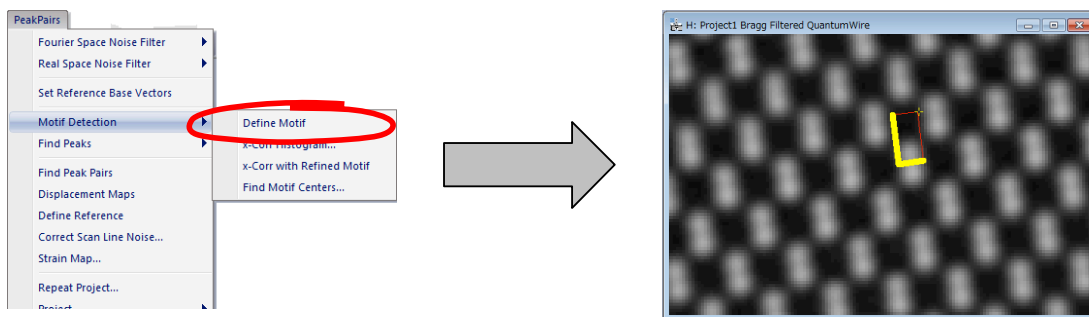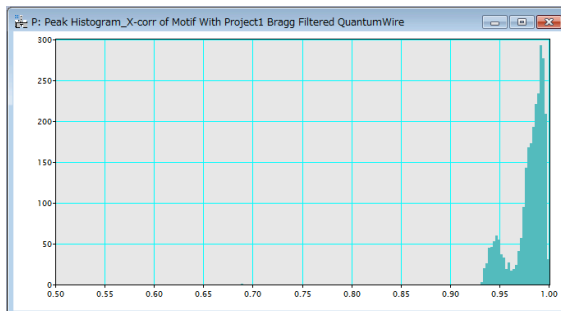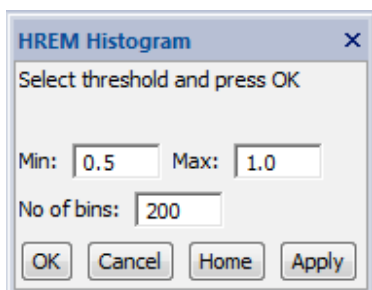

Once the Motif has been defined, select the **x-Corr Histogram** in the Motif Detection submenu. A dialog shown below will open:
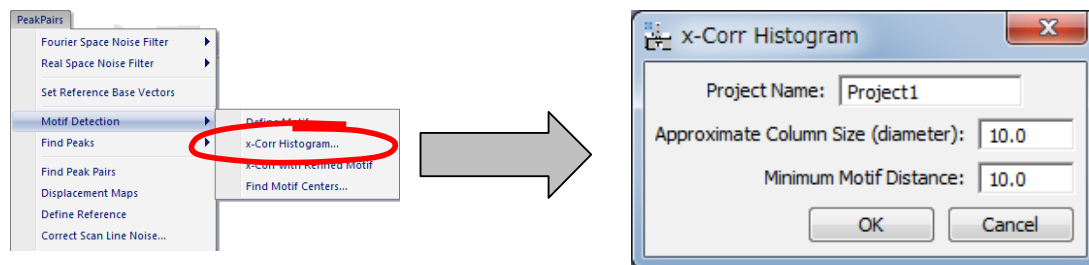

After clicking OK, the HREM Histogram tool shown below and a new window will appear showing the histogram of all maxima found in the Cross-Correlation map, obtained using the *User-Selected* motif and the whole image.

HREM Histogram tool

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, just click the mouse on the histogram, and select the desired range of peaks.
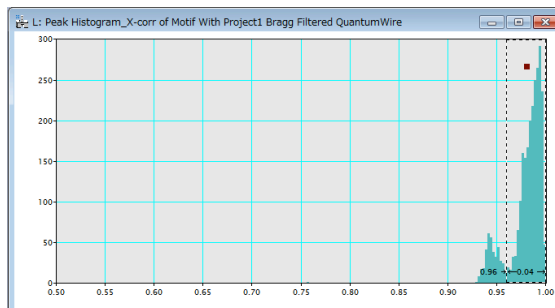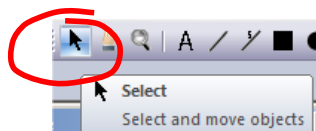
The discovered motifs will be classified to red or blue depending on their cross-correlation values: red indicate the motif, whose cross-correlation value is higher than the selected threshold, while blue indicate the motif equal to or lower than the threshold. The peak color will be dynamically revised by changing the threshold.
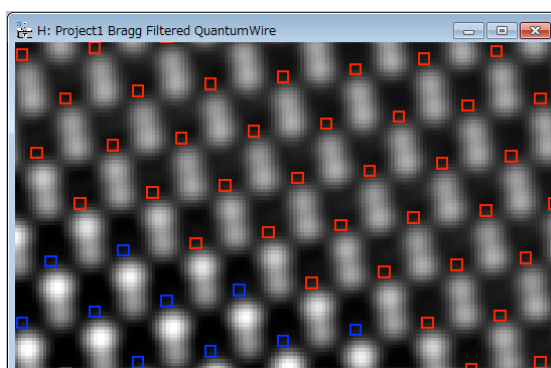

Given that we are interested in the detection of both cations, we will select a threshold lower than 0.9 to take all peaks into consideration. To do that, the **Select** tool should be used by dragging the mouse on the histogram directly. The left edge will be used as a lower threshold.
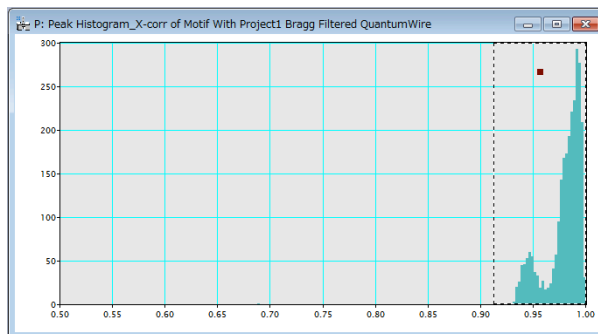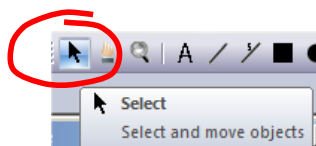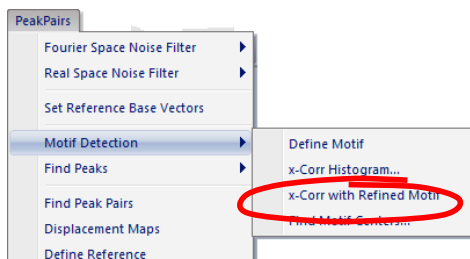
When you satisfy the threshold by looking the motif markers (red or blue), push the "OK" button of the Histogram tool, or the "Cancel" button to stop the process.

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 average motif is automatically shown:
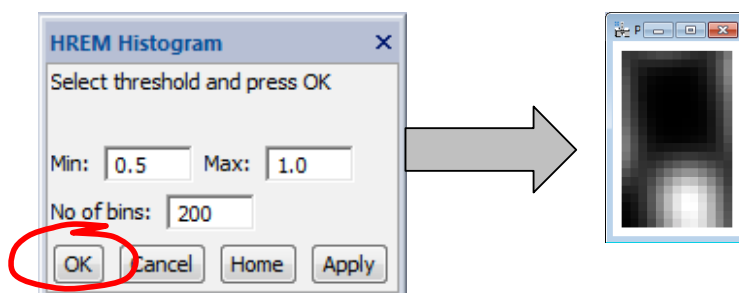
The second step of the Motif detection is calculating the cross-coefficients using the refined motif. To do so, select the **x-Corr with Refined Motif** command.

Then, this command will show the HREM Histogram tool and the cross-correlation between the refined Motif and the whole image. This is especially useful in the presence of noise.
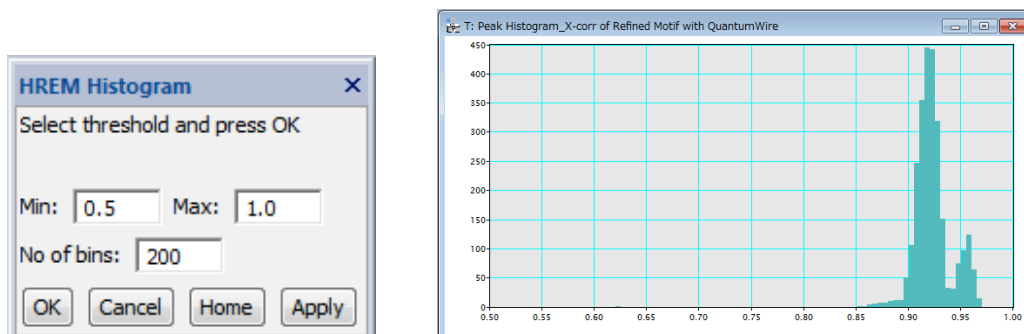
Once the refined histogram is shown, the user should select the intensity threshold on the refined histogram as before.
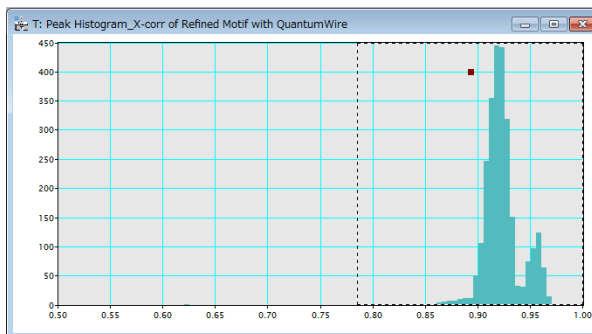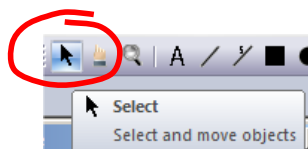
The discovered motifs will be classified to red or blue as before. The peak colour will be dynamically revised by changing the threshold. When you satisfy the threshold by looking the motif markers (red or blue), push the "OK" button of the Histogram tool. Then, the second refined motif will be shown.
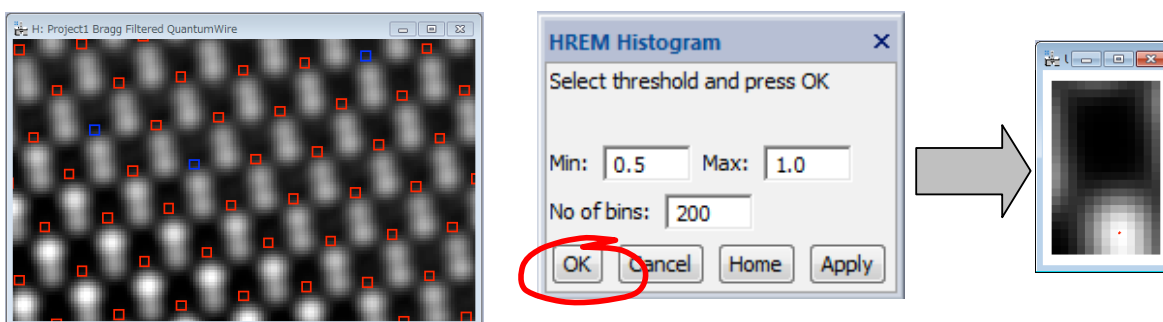
The final step of the Motif detection is finding the motif centers. To do so, select the *Find Motif Centers* in the Motif Detection submenu.
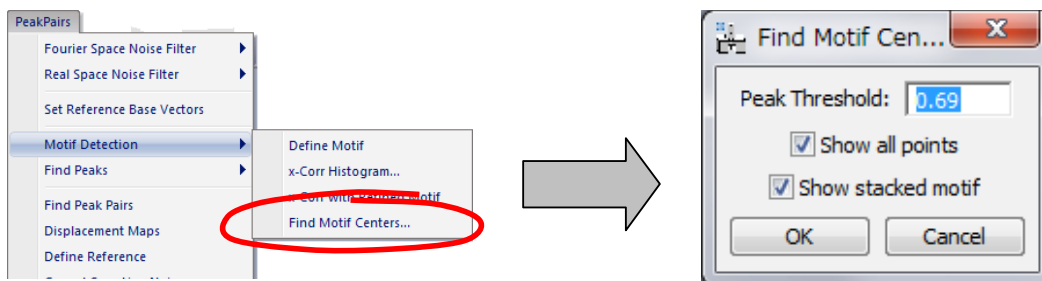
The **Find Motif Centers** command finds the motif positions by taking into account the minimum motif distance, and places the *red* small boxes on the motif centers (the center of the motif box).
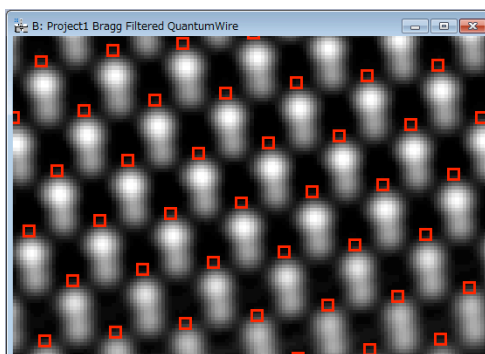
IMPORTANT: In the case of Motif Detection, the reference base vectors should be selected using the **Set Reference Base vectors** before applying the **Find Peak Pairs** command.

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.
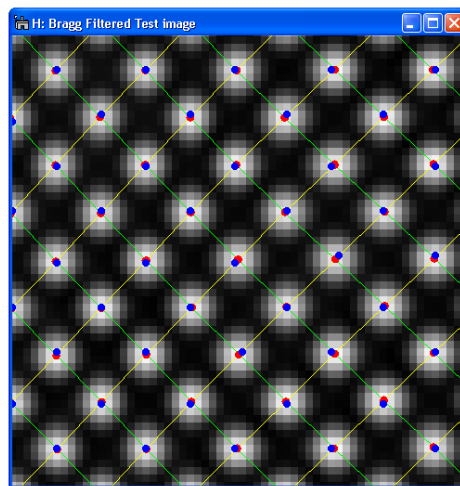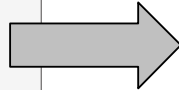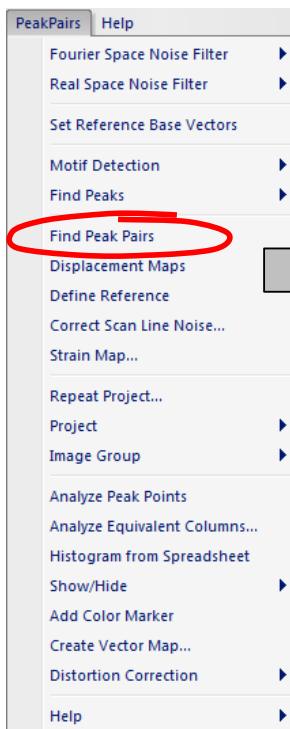
Peak Finding
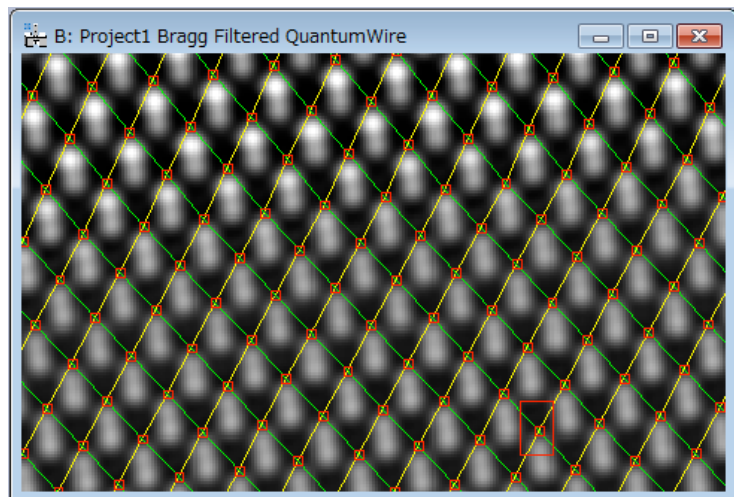
Motif Detection

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).
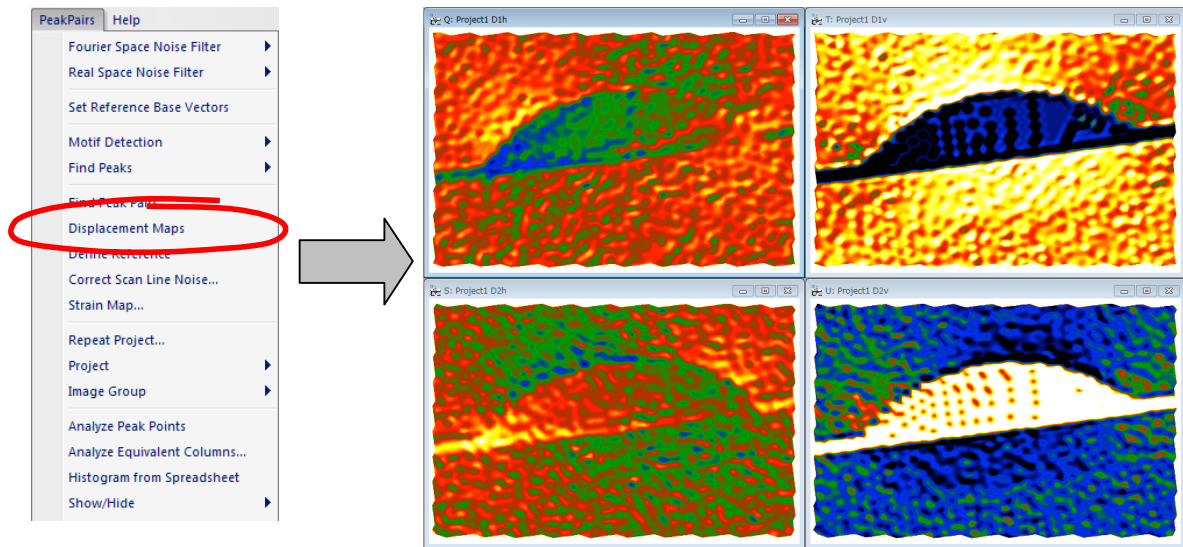
Technical note:

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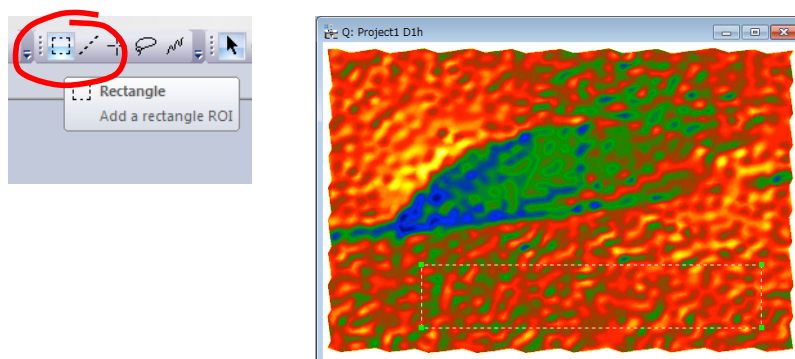
Once the Rectangle ROI has been placed, the user should select the **Define Reference** command. This will change the displacement values, so as to obtain a uniform displacement in the chosen reference area.

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

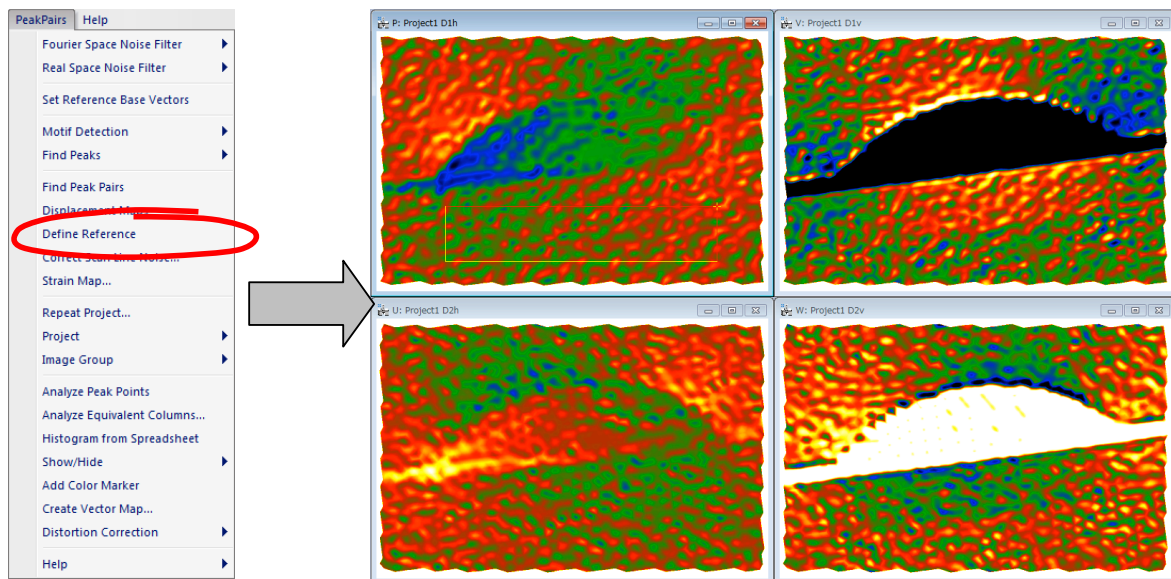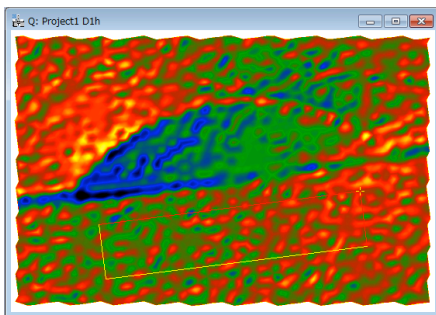You can adjust the edge length by selecting the yellow edge and dragging the handle, and rotate the ROI by dragging the yellow cross (+).

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.
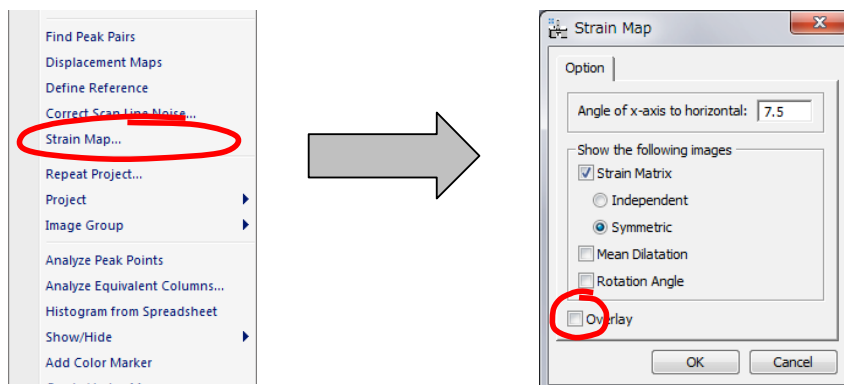
The angle of x-axis to horizontal may be determined graphically. To do so, just add a **Line ROI** on the original image, along the desired direction of x-axis, *before issuing* the **Strain Map** command.
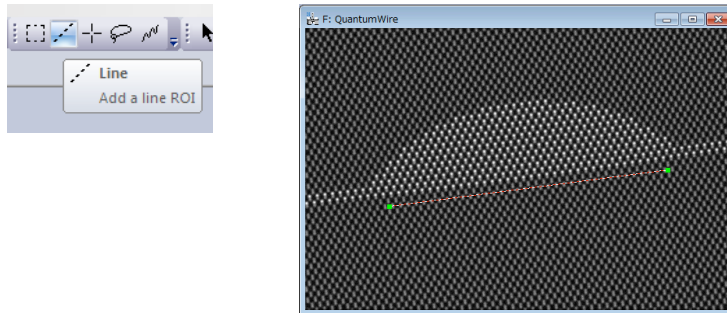
Once the OK button is chosen, a set of 4 images corresponding to (e_{xx}, e_{yy}, e_{xy} and e_{yx}) are obtained. The mean dilatation and Rotation angle are additional images available.

There is an option for strain representation (Overlay):

DESCRIPTION	*Full image*	*Detail*
No overlay: Continuous strain maps are shown. **Hint:** If you prefer a grey scale or a different contrast limit, press the right button on the image, and modify ImageDisplay options properly.		
Overlay: Strain maps at each atomic column are shown with colour dots over the original images.		

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->2and 1->3.
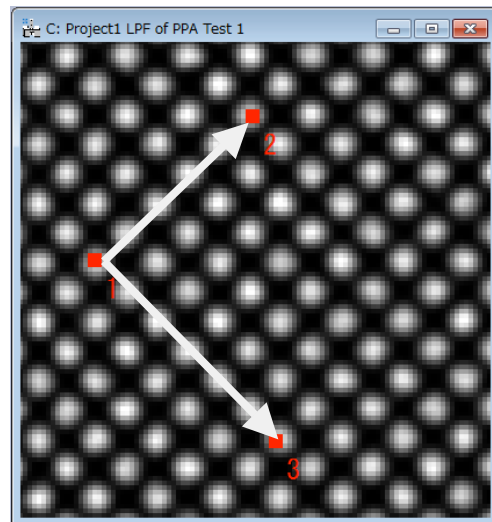
Approximate directions
as described by the user

When applying the **Set Reference Base Vectors** command, 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->2and 1->3.
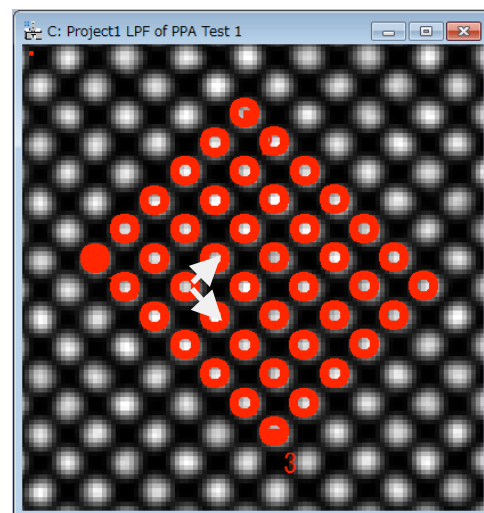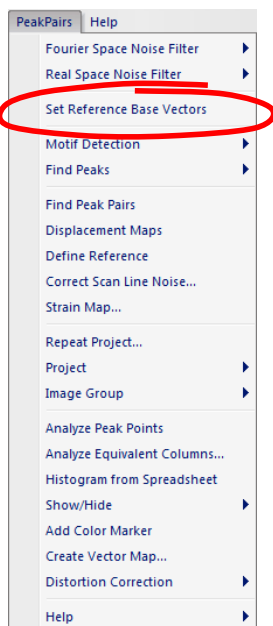
Reference Base Vectors

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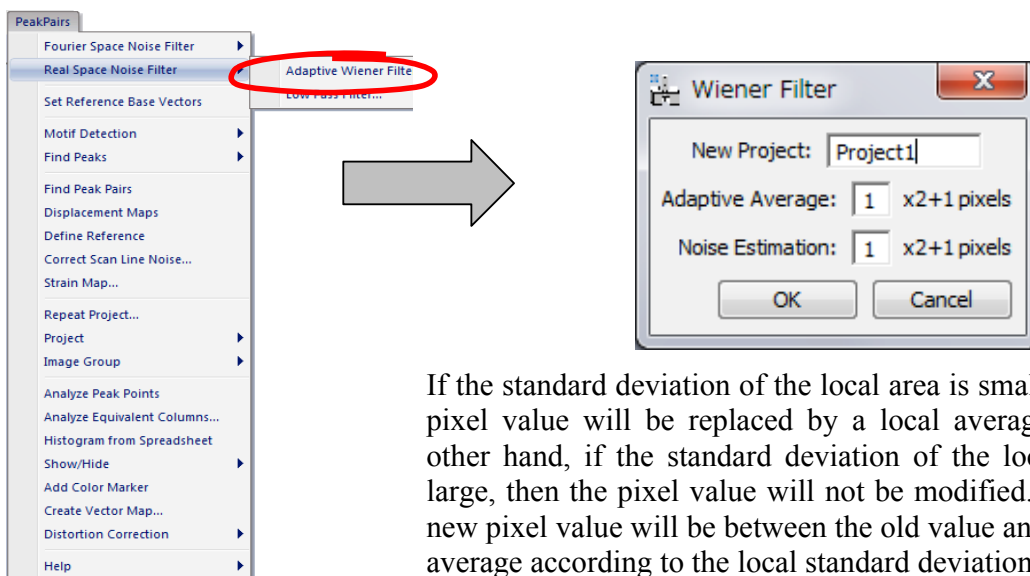
If the standard deviation of the local area is small, then the pixel value will be replaced by a local average. On the other hand, if the standard deviation of the local area is large, then the pixel value will not be modified. Thus, the new pixel value will be between the old value and the local average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

The result of the Wiener filtering operation on *Test image.dm3* (Adaptive Average =3, Noise Estimation=3) is depicted below.
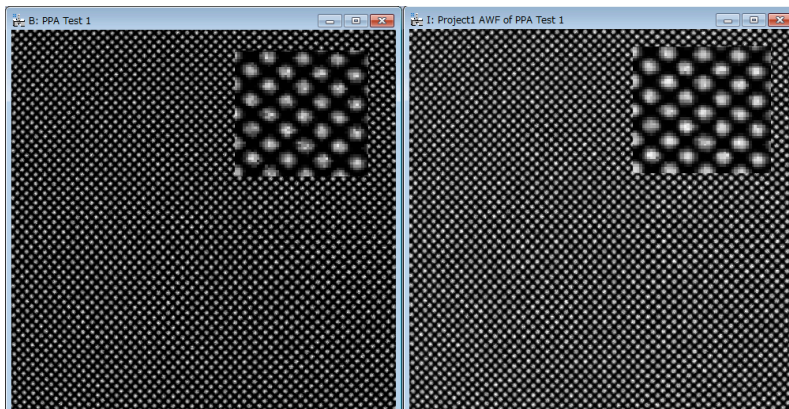
Low Pass Filter

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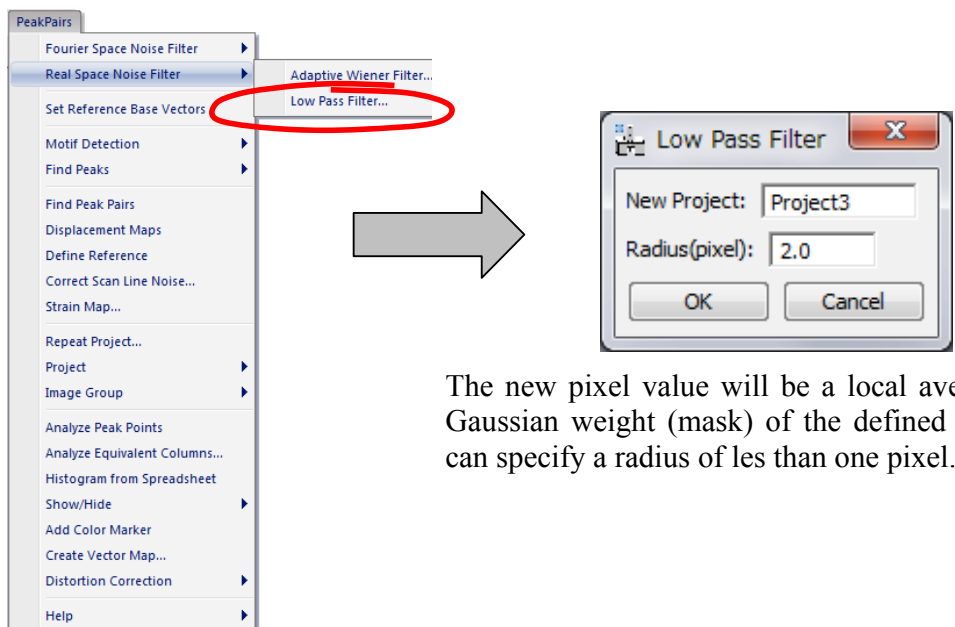
The new pixel value will be a local average with a Gaussian weight (mask) of the defined radius. You can specify a radius of les than one pixel.

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) |
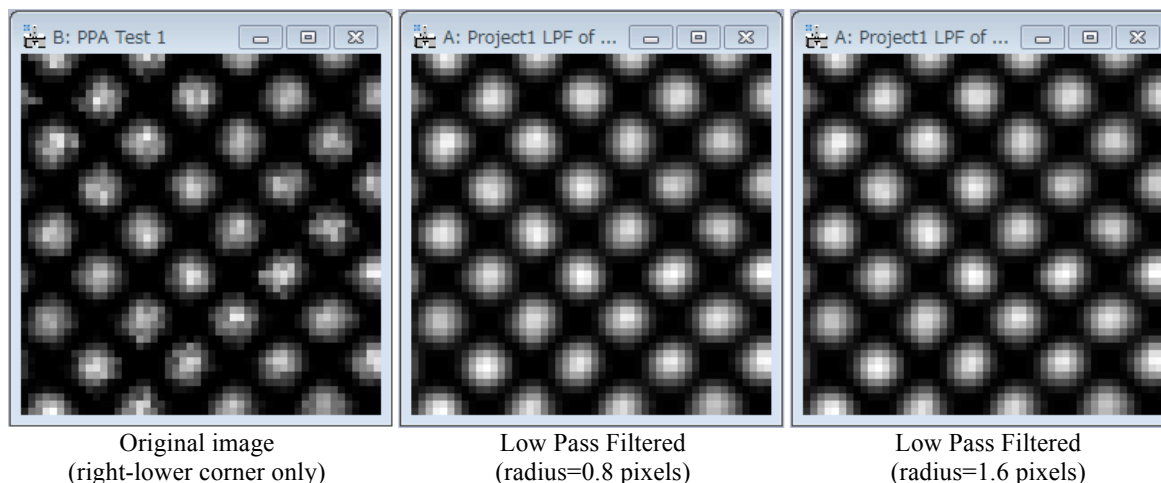
Geometric distortion correction

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.

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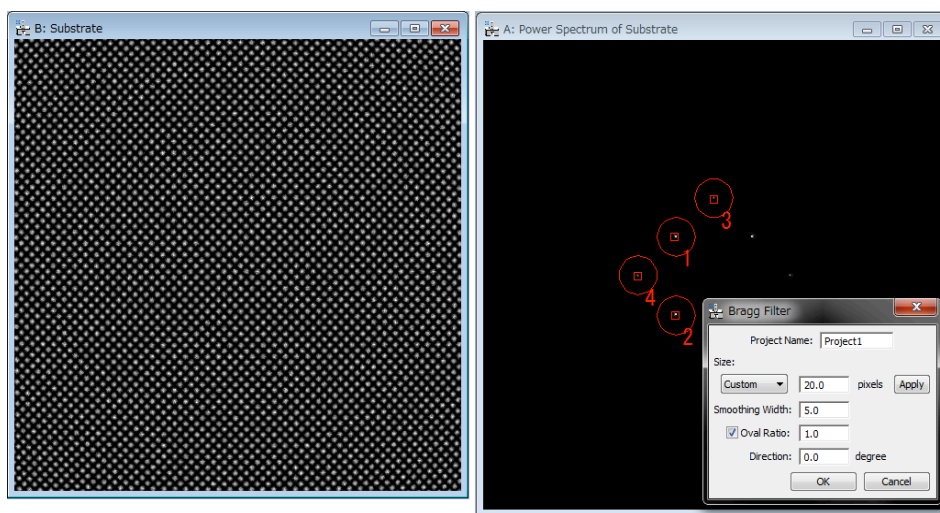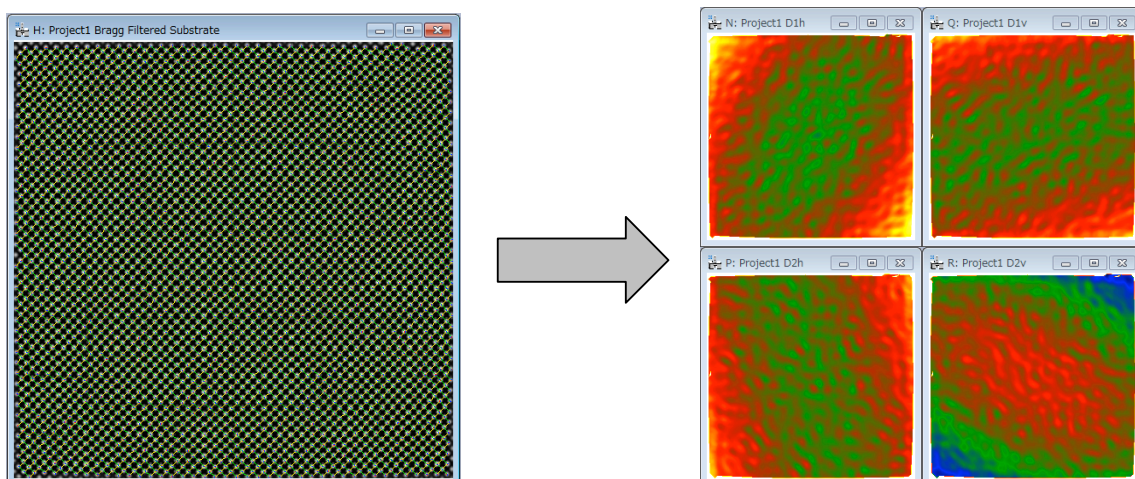
The distortion information obtained for the perfect crystal image can be used to correct distortions in any other image with the same distortion. In order to obtain the distortion information, select the image with *Peak Pairs* information, and apply the command **Obtain Distortion Info**.
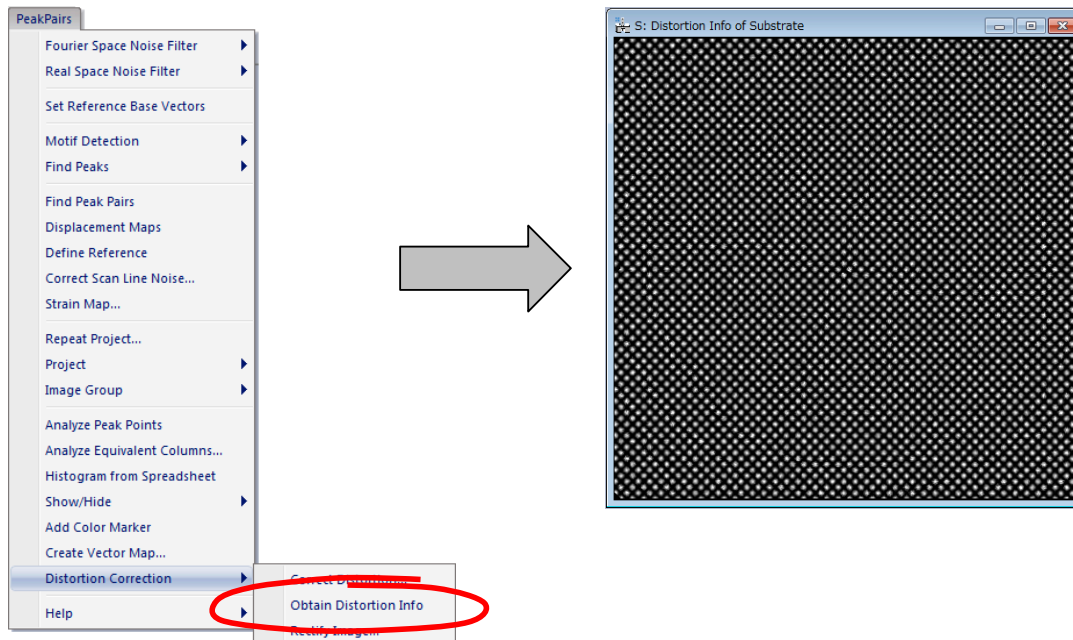
The new image with distortion information will be created. This *Distortion Info* image can be saved to disk (e.g., *Distortion Info of Substrate* using **Save As** command) and used in further analysis of the image having the same distortion.

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:
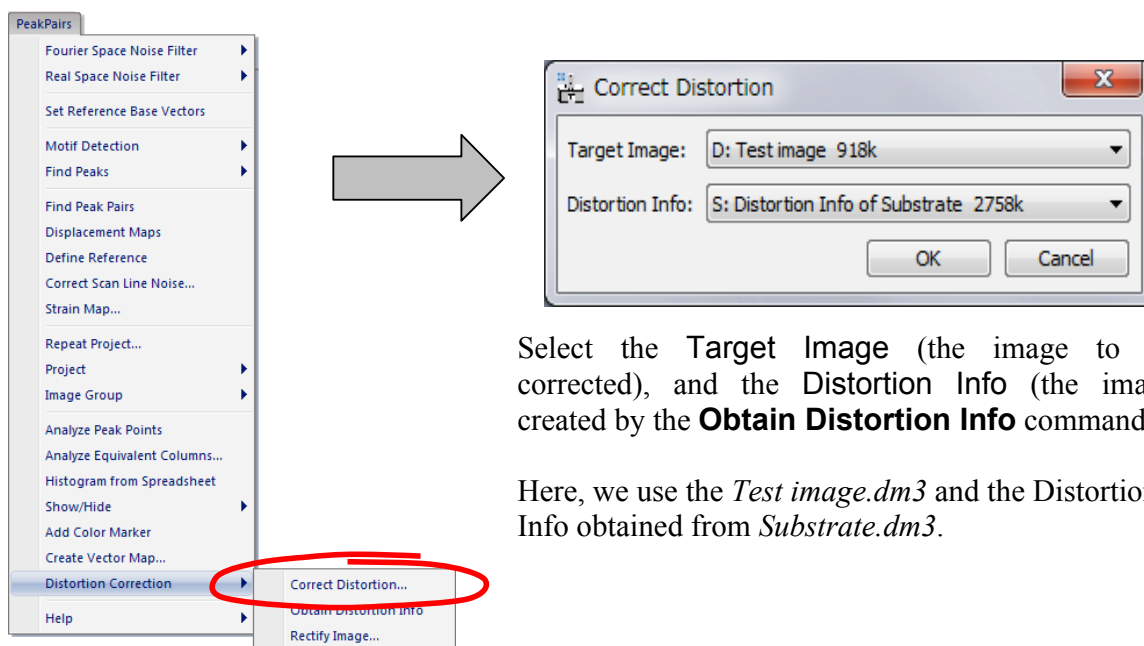
Select the Target Image (the image to be corrected), and the Distortion Info (the image created by the **Obtain Distortion Info** command).

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
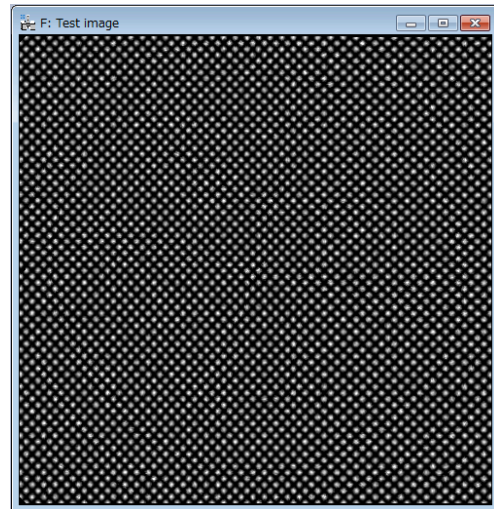
The strain maps before and after distortion correction:

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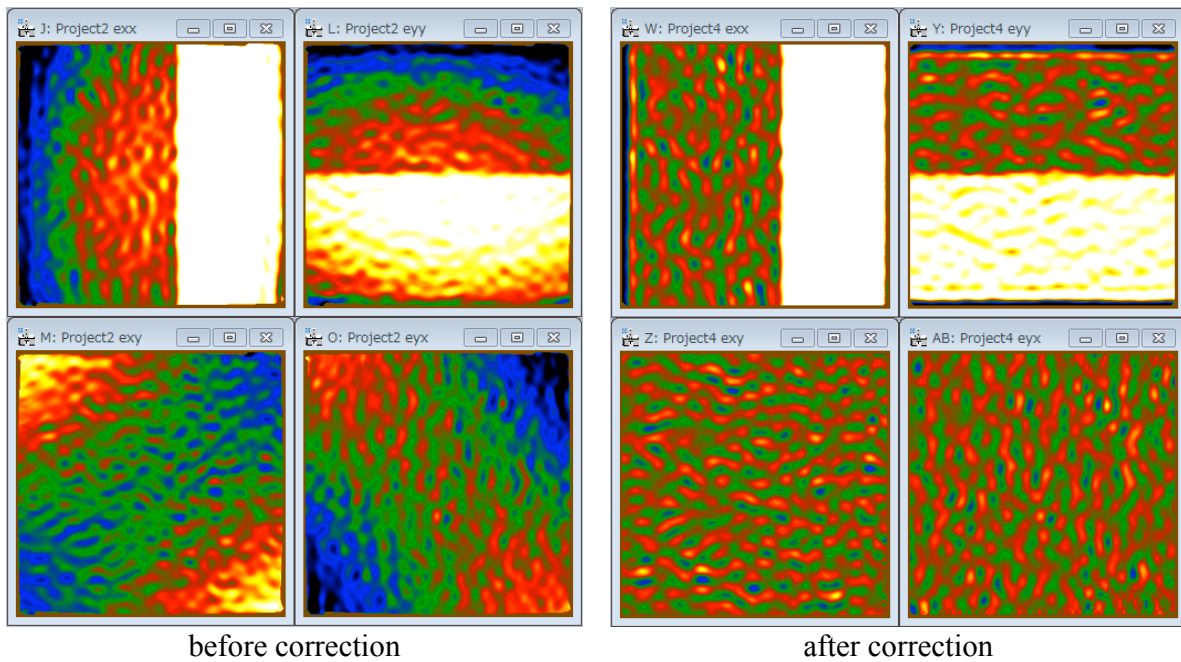
If we plot a horizontal profile across exx and a vertical one across eyy, we get the expected results (exx=0.1 and eyy=0.05) after distortion correction.
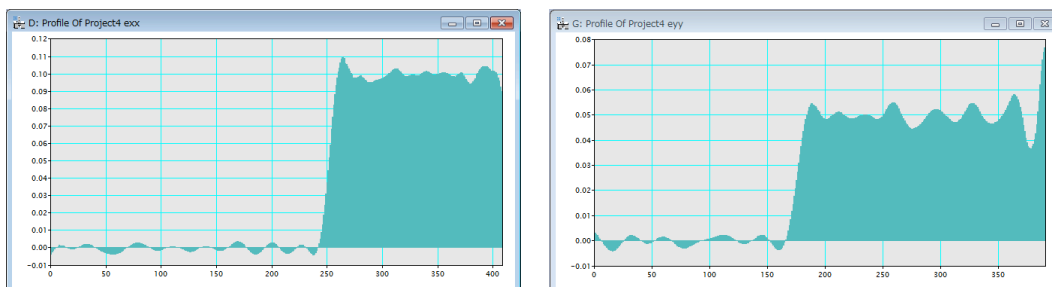
Additional functions

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.
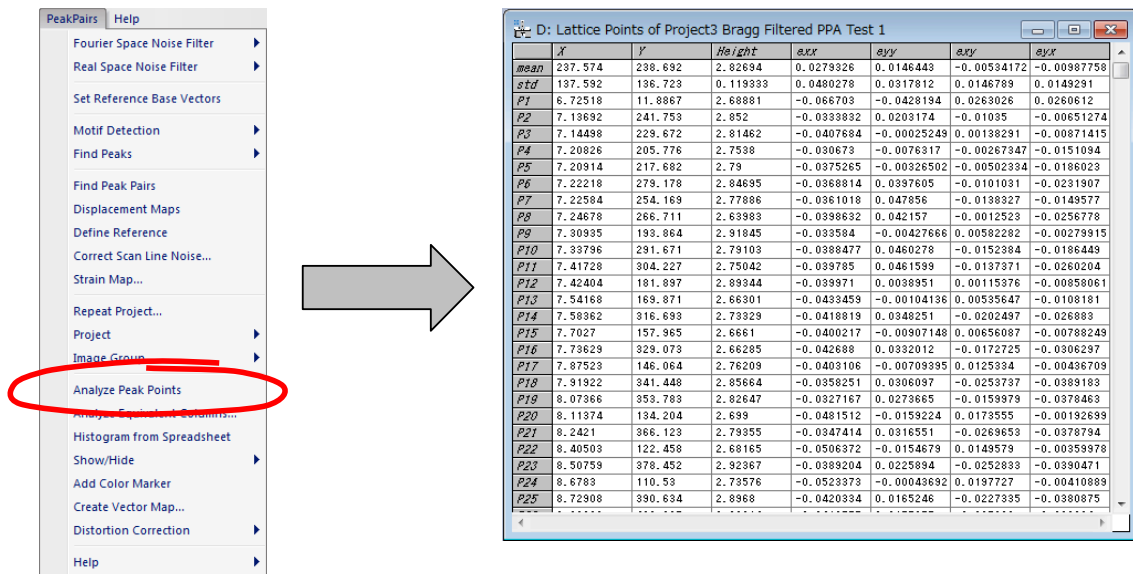
It is also possible to get a histogram from the Spreadsheet by using the **Histogram from Spreadsheet** command, thus obtaining a different histogram for each column in the spreadsheet.
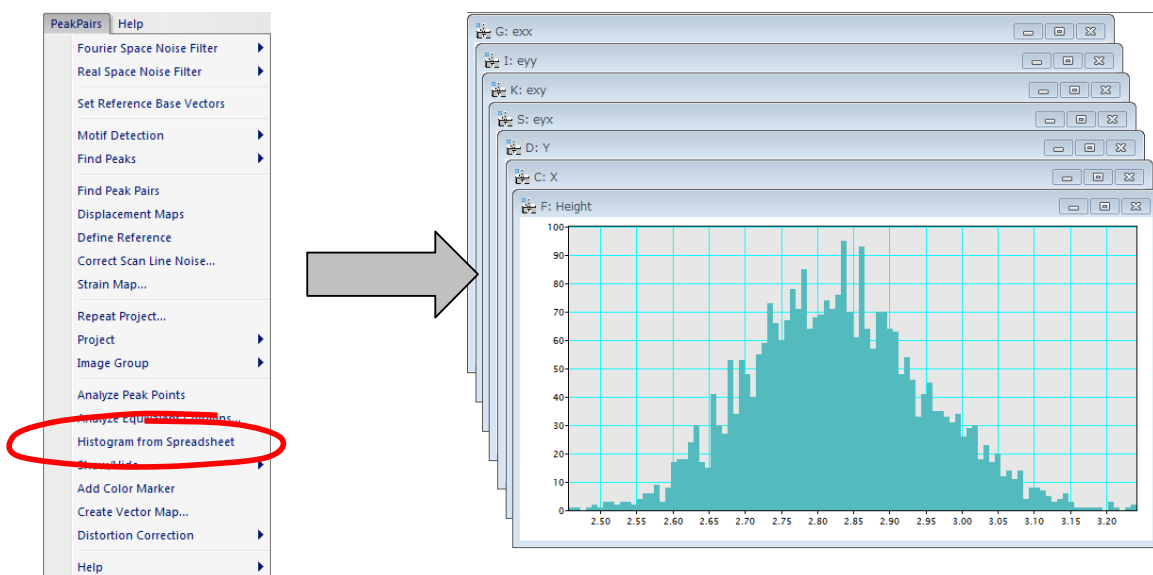
Atomic Column Analysis (Analyze Equivalent Columns)

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
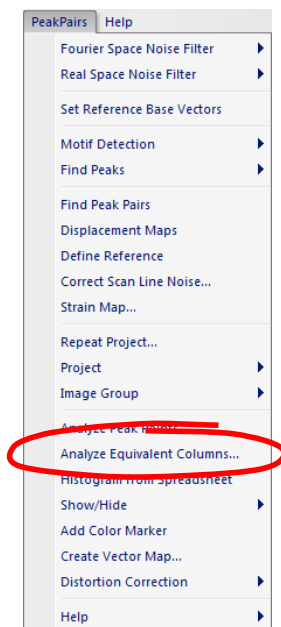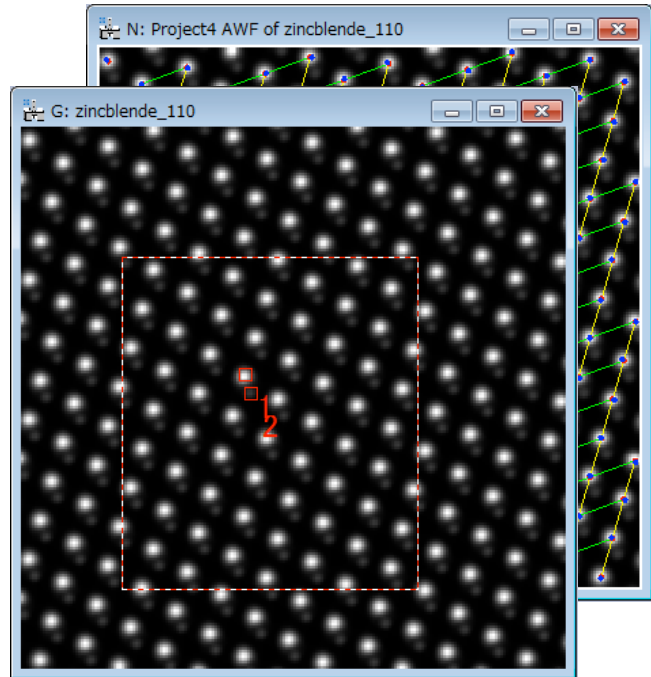
All the columns in the selected area will be shown in the image, and the intensity of each column will be stored in a spreadsheet.
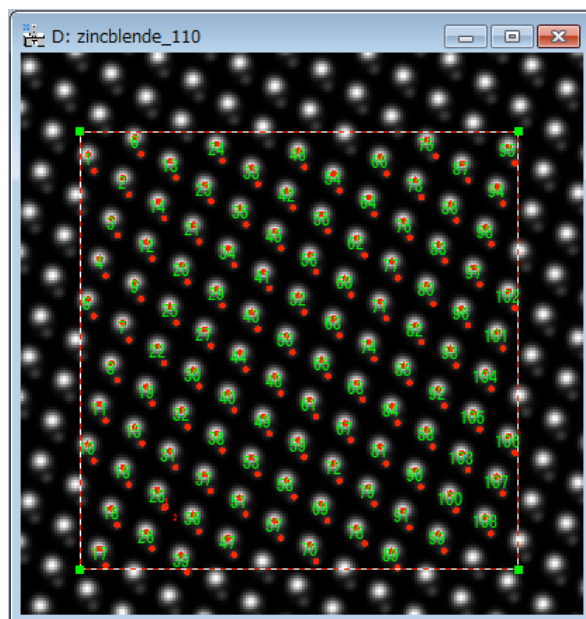
U: Distance_zin...	1-2
mean	6.36442
std	0.0886919
Pos1	6.36691
Pos2	6.36616
Pos3	6.37164
Pos4	6.40395
Pos5	6.38842
Pos6	6.34961
Pos7	6.37638
Pos8	6.40828
Pos9	6.374
Pos10	6.37056

AD: Peak_zincblende_110

	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.
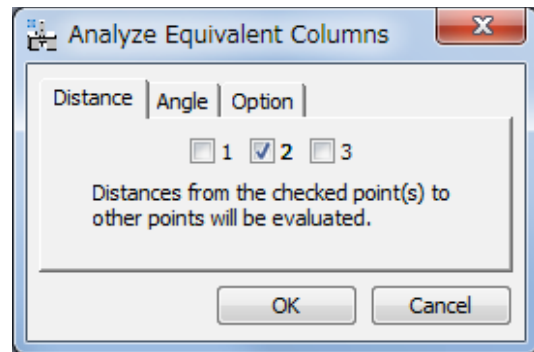
If there are more than two columns, the user will have the option to evaluate the angles subtended by two neighbour columns.
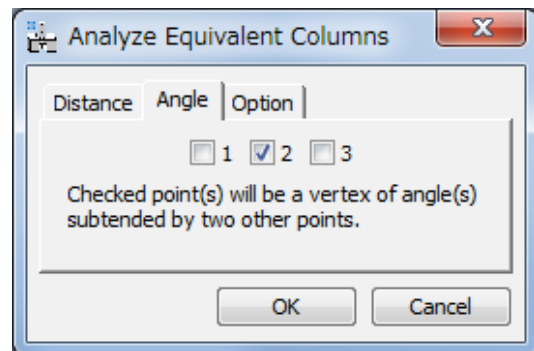
You can see visually the distribution of distances using the **Histogram from Spreadsheet** command:
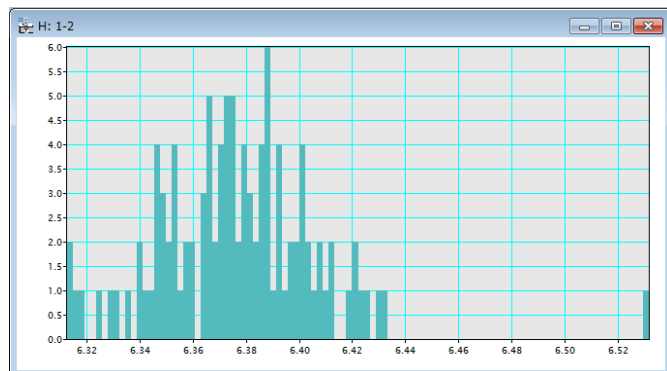
Correct scan line noise

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:
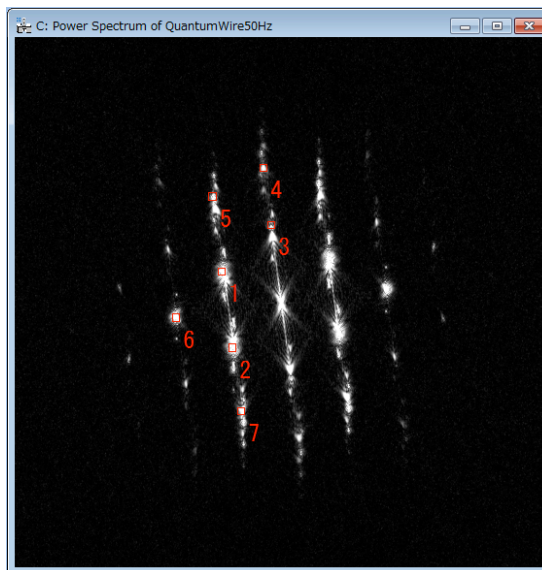
If we specify the lattice base vector (#1 and #2 as indicated), displacement maps shown below may be obtained. As we may observe, a set of stripes is shown in these maps:
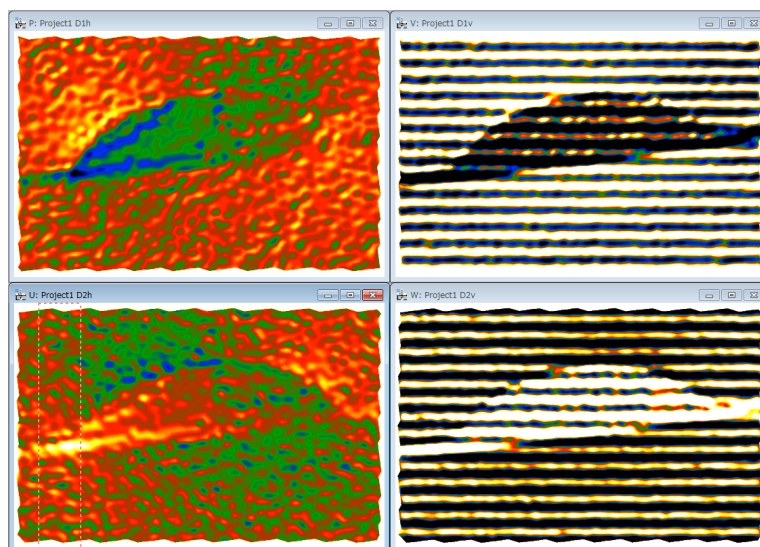
We can then Add a Rectangle ROI in one of the Displacement maps (here, the image U).
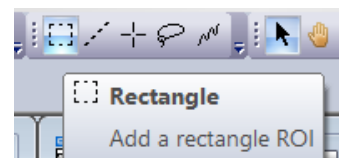
Then, press the **Correct Scan Line Noise** option to remove the stripes and determining a proper displacement map.
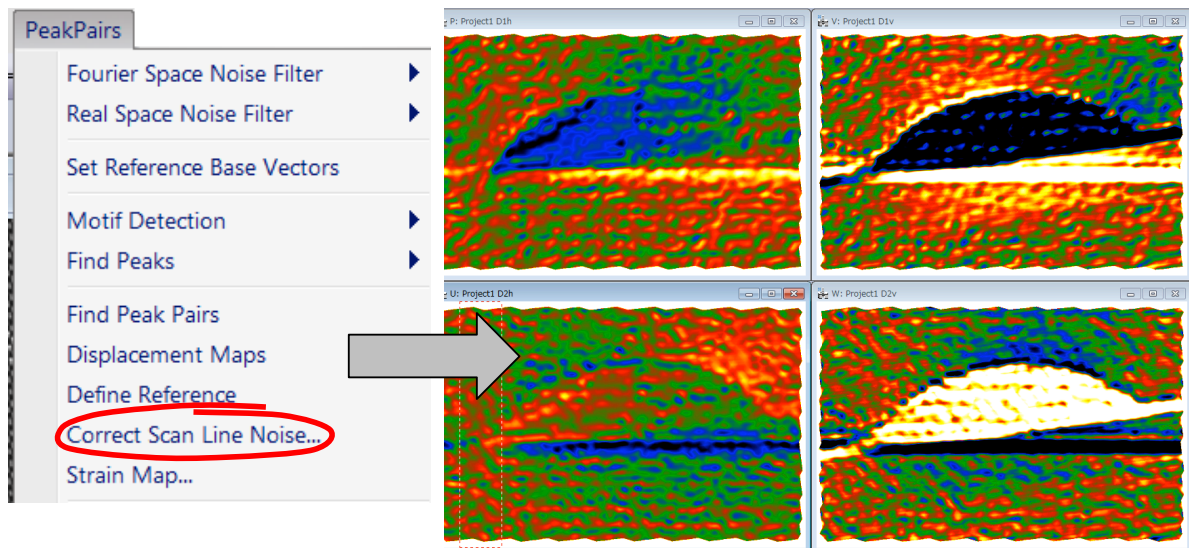
You can extend the reference area for the scan-line correction from the very top to the bottom lines, when you check "Correct All Line" in the dialog.
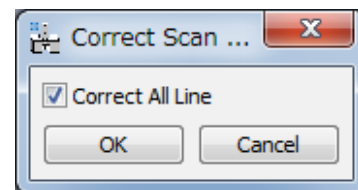
Unfortunately, in this example there is no perfect reference area from the top to bottom of this image. Therefore, we have horizontal artefacts as clearly see in the images V and W.

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.
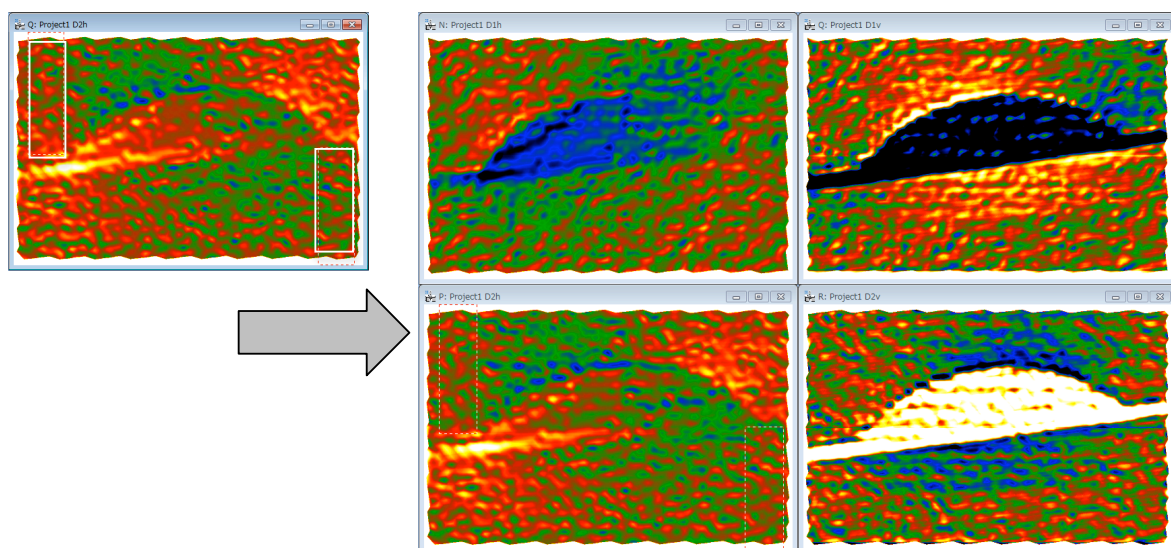
Create Vector maps

It is possible to a create 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.
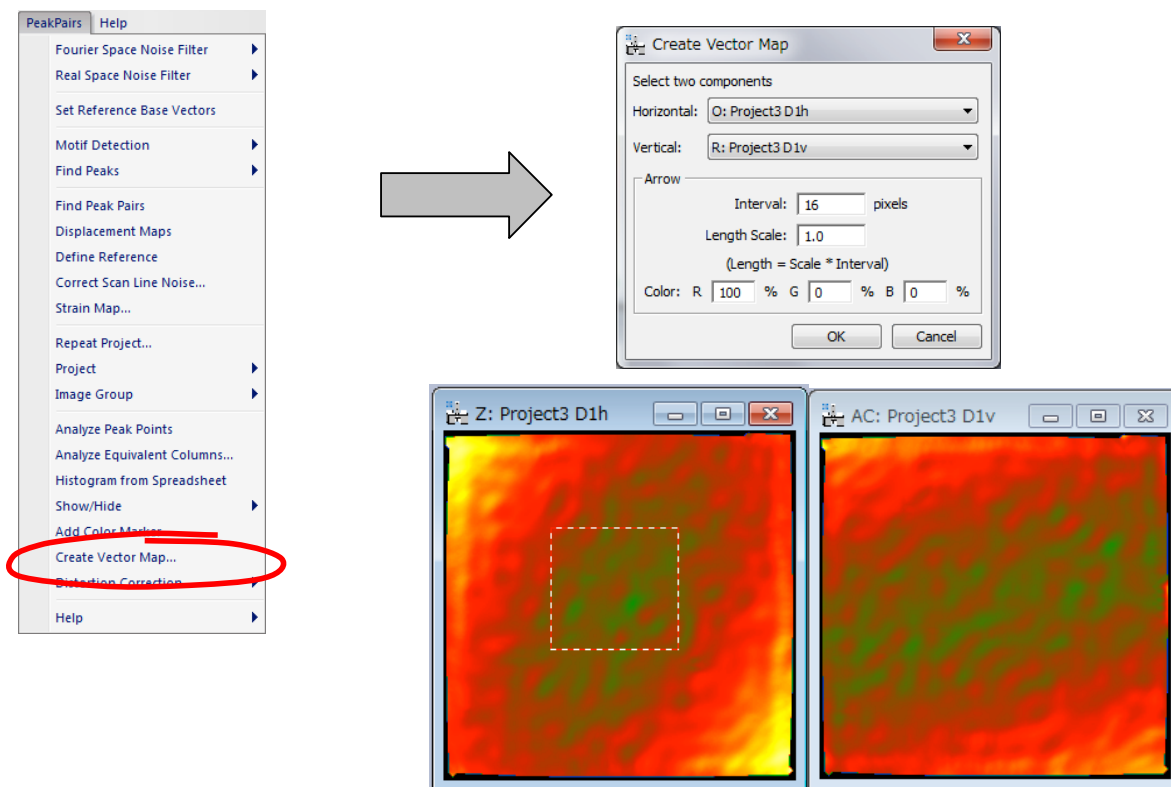
Then, you will get a colour map corresponding to the vector magnitude, with arrows showing the directions and magnitudes of the vectors as shown below:
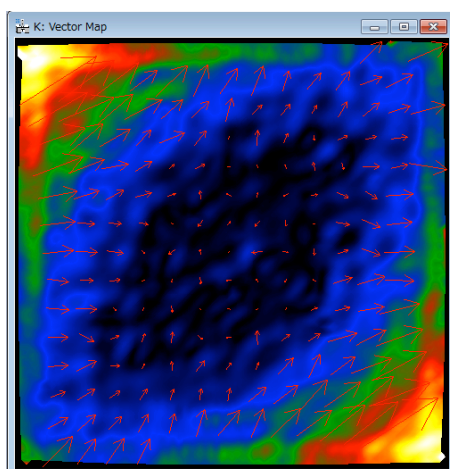
The vector map here is a complex DM image, whose real and imaginary parts correspond respectively to the Horizontal and Vertical images selected in the dialog.

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.
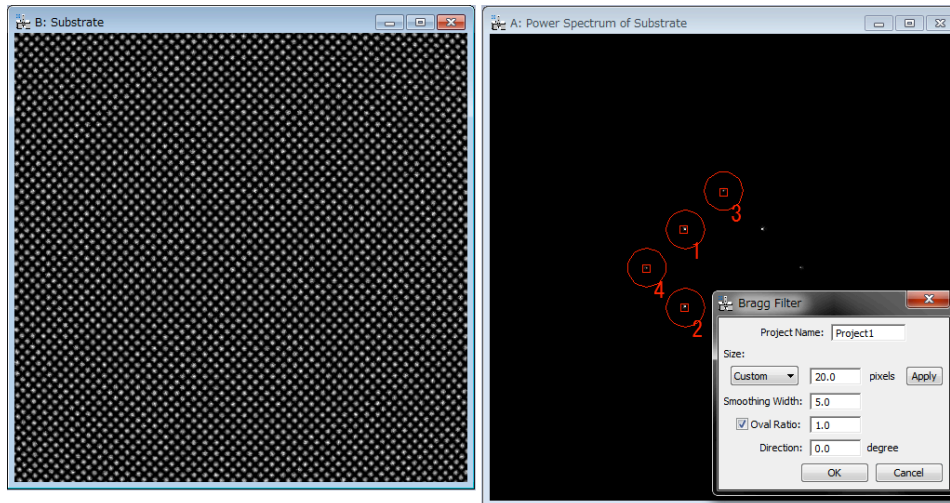
Then calculate the *Peak Pairs* using the usual commands (**Find Peaks** followed by **Find Peak Pairs**). If we analyse the displacements with the **Displacement Maps** command, we can observe that the image of a perfect crystal is distorted as shown below.
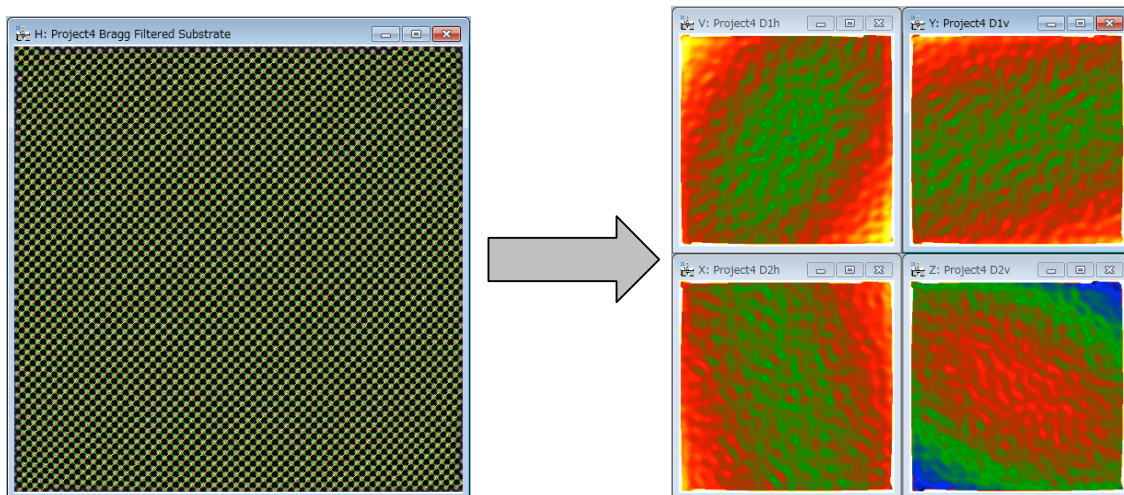
Given that the image corresponds to a perfect crystal, we can get a rectified image. In order to do that, select the project image with Peak Pairs information, and then apply the **Rectify image** command.
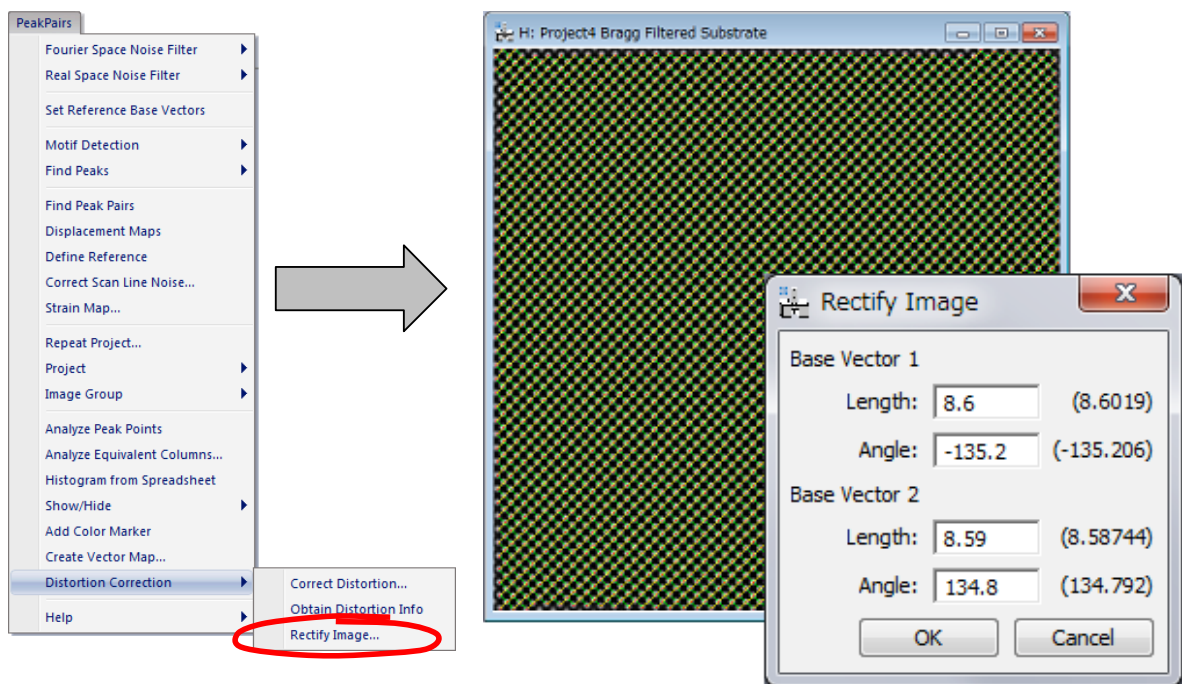
The lengths and angles of current reference base vectors will be shown in the dialog. If the values in the parentheses differ from the values expected from an ideal unit cell, you can change the values accordingly.

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:

before correction   after correction
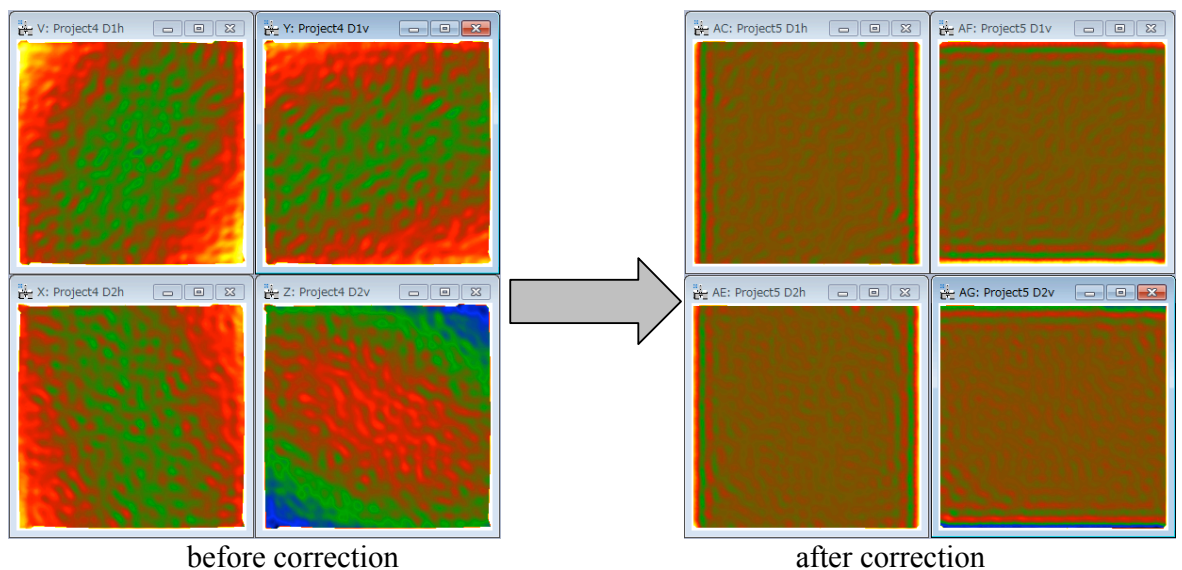
Appendix

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 :

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

Rotation (in radians and anti-clockwise positive):

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

Some useful DM tricks

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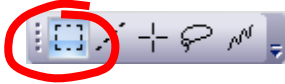
> **Hint:** to select a square area, hold down SHIFT. To select powers of two, hold down SHIFT-ALT.

DM Zoom tool:
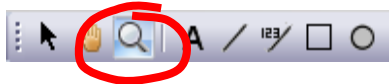
> **Hint:** to demagnify, press ALT.

HREM Mouse tool
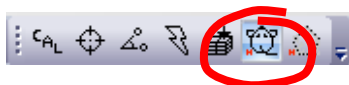
> **Hint:** to delete any spot, just click on the mouse mark with the SHIFT key down.

DM Image Display Command
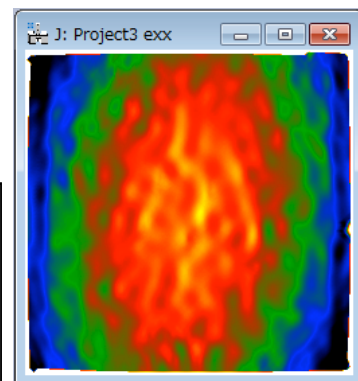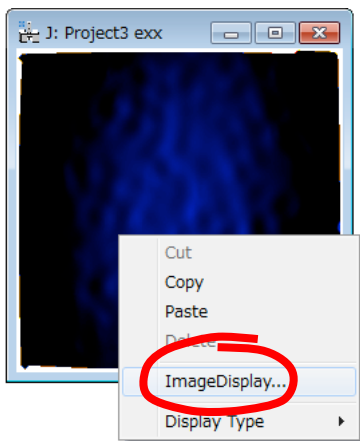
> **Hint:** to change the color map of any image, press the right mouse button on it, select ImageDisplay, and modify the options as desired.
>
> For example, it is useful to set manually the color range of each map to be the same, so as to be able to compare each other.

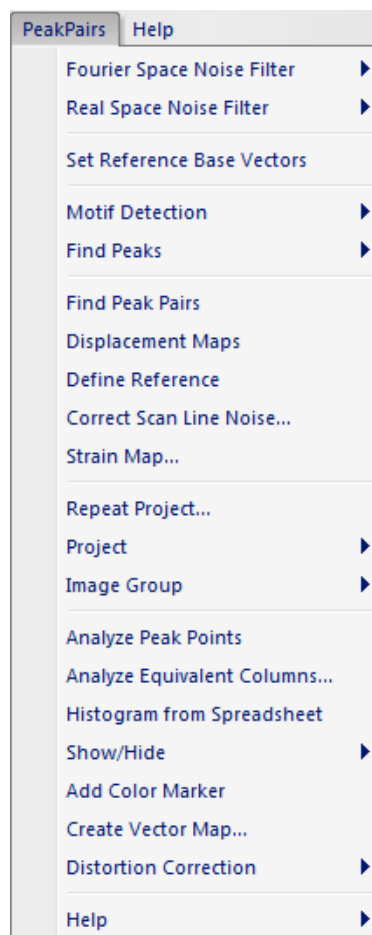|	
Find Peaks (see sub menus)	Locates peaks of intensity in an image. Note: Reference base vectors should be defined beforehand.
Find Peak Pairs	Calculates pairs of peaks along two reference base vectors automatically.
Displacement Maps	Generates horizontal and vertical displacements along the two directions 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.
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

Power Spectrum

Bragg Filter...

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

Bragg Filter

Project Name: Project1

Size:

Custom ▼ 20.0 pixels Apply

Smoothing Width: 5.0

☑ Oval Ratio: 1.0

Direction: 0.0 degree

OK   Cancel
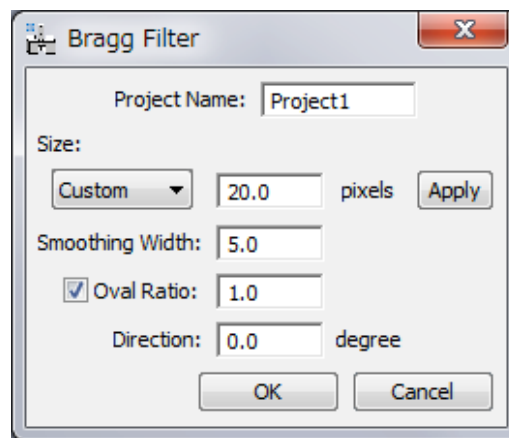
Component	Description
Project Name	Name given to the group of images and results
Size	Defines mask radius of hard cut-off (beyond which values are set to zero).
Smoothing Width	Specifies mask smoothing width in pixels
Oval Ratio	Defines the shape of the oval, as major to minor axis ratio
Direction	Sets the prescribed masks angle, in degrees

Real Space Noise Filter SubMenu

Adaptive Wiener Filter...

Low Pass Filter...

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

Wiener Filter

New Project: Project1

Adaptive Average: 1 x2+1 pixels

Noise Estimation: 1 x2+1 pixels

OK   Cancel
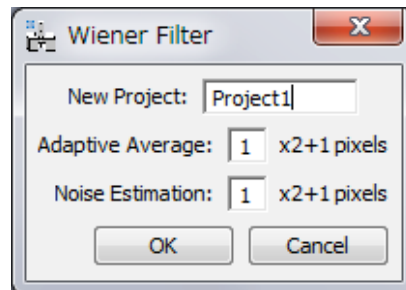
Component	Description
New Project	Name given to the group of images and results
Adaptive Average	Window size [(2N+1)x(2N+1) pixels] to be used in the calculation of the adaptive average
Noise Estimation	Window size [(2N+1)x(2N+1) pixels] to be used in the calculation of the noise estimation
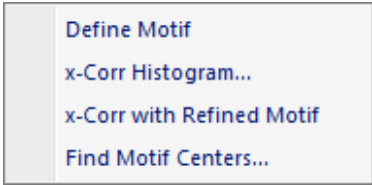
Low Pass Filter Dialog

Dialog

Low Pass Filter

New Project: Project1

Radius(pixel): 2.0

OK   Cancel
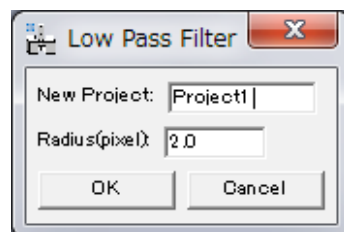
Component	Description
New Project	Name given to the group of images and results
Radius(pixel)	The radius of the mask in pixels

Motif Detection SubMenu

| | Define Motif |
| x-Corr Histogram... |
| x-Corr with Refined Motif |
| Find Motif Centers... |

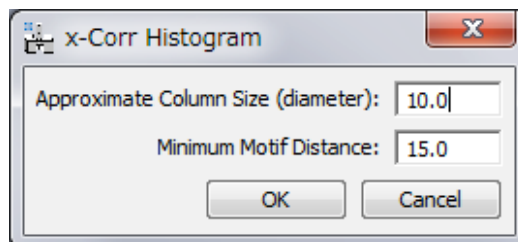| Component	Description
Define Motif	Define a Rectangle ROI as a Motif, and make it rotatable.
x-Corr Histogram… (see Dialog)	Calculates Cross-Correlation Histogram between the selected reference region (motif) and the original image. Note: The left edge of the selection in the histogram is used as a threshold to obtain the refined motif in the next step.
x-Corr with Refined Motif	Obtains a refined motif, and then calculates Cross-Correlation Histogram between the refined motif and the original image. Note: The left edge of the selection in the histogram is used as a threshold to find good motifs in the next step.
Find Motif Centers... (see Dialog)	Finds the centers of good Motifs in the image.

x-Corr Histogram Dialog

Dialog

x-Corr Histogram

Approximate Column Size (diameter): 10.0

Minimum Motif Distance: 15.0

OK   Cancel

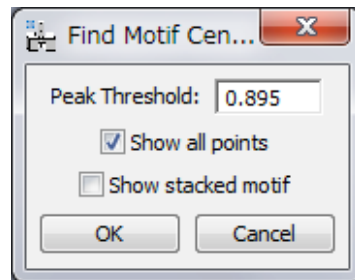| Component	Description
Approximate Column Size (diameter)	Specifies an approximate atom column size (the minimum distance between atom column peaks). (This parameter is used in **x-corr with Refined Motif** to define peaks in the refined motif.)
Minimum Motif Distance	Specifies a minimum distance between allowed motifs. (This parameter is used in **Find Motif Centers…**)

Find Motif Center Dialog

Dialog

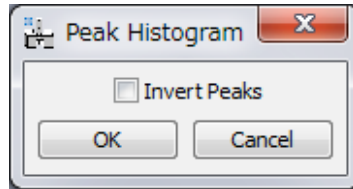| Component	Description
Peak Threshold	Specifies a minimum for the intensity of allowed Peaks.
Show all points	Shows also the Motif centers in blue that were rejected by the cross-correlation threshold and/or the minimum motif distance criteria. (Namely, all the peak points are displayed in red or blue color.)
Show stacked motif	Make a stacked image from detected motifs.

Find Peaks SubMenu

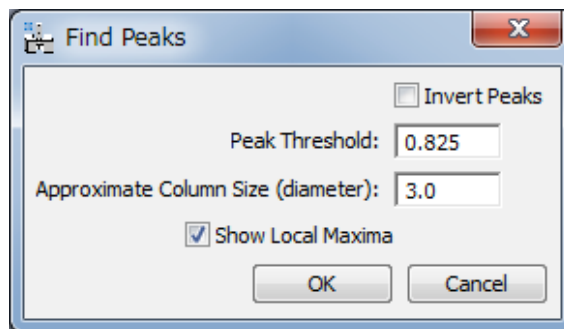| Component	Description
Peak Histogram... (see Dialog)	Calculates a histogram of peaks intensities, helping the user to determine a precise value for Peak Threshold.
Find Peak Positions… (see Dialog)	Locates peaks of intensity in a filtered image. A threshold for the minimum allowed peak intensity and a minimum distance for peaks can be defined. Note: The left edge of the selection in the histogram is used as a threshold to find good peaks. This threshold can be changed in the dialog below.
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**.

Peak Histogram Dialog

Dialog

Component	Description
Invert Peaks	It allows the user to calculate intensity minima histograms (instead of maxima)

Find Peak Positions Dialog

Dialog

Component	Description
Invert Peaks	It allows the user to calculate intensity minima (instead of maxima)
Peak Threshold	Specifies a minimum for the intensity of allowed peaks
Approximate Column Size (diameter)	Specifies an approximate column size (in pixels) to merge the peaks (columns) within the specified column size.
Show Local Maxima	Show local maxima (of 8-neighbourhood) as blue points.

Correct Scan Line Noise Dialog

Dialog

Component	Description

HREM Research Inc
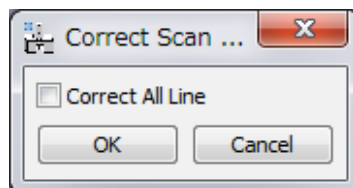
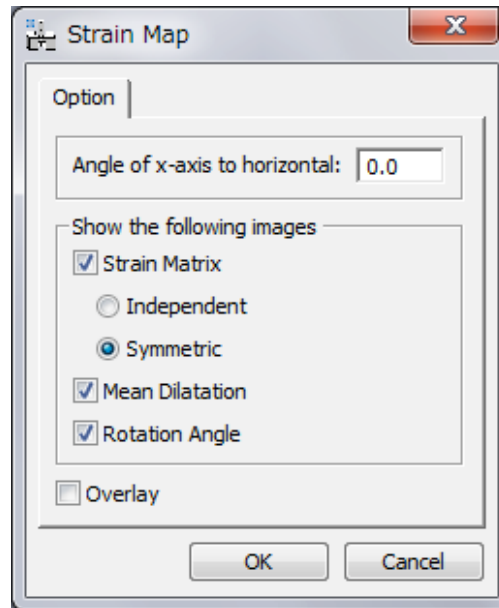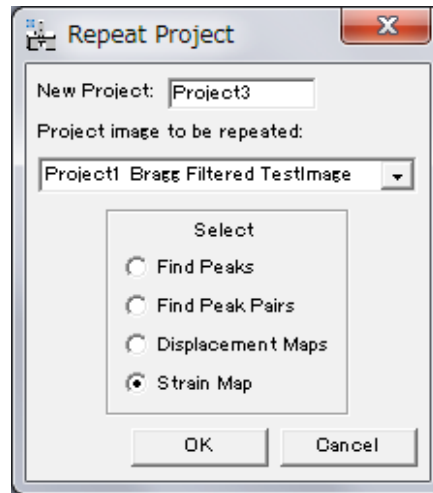| Correct All Line	It modifies all scan lines, not only those within the ROI.

Strain Map Dialog

Dialog

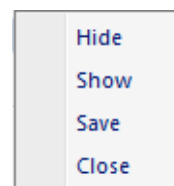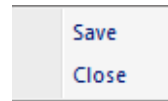| Option	Description
Angle of x-axis to horizontal	Specifies the angle of the direction to be considered as x-axis. You can specify the orientation of the x-axis by placing a Line ROI on the HREM image. In this case, the angle of the Line ROI appears here automatically. Note: If angle is set equal to 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

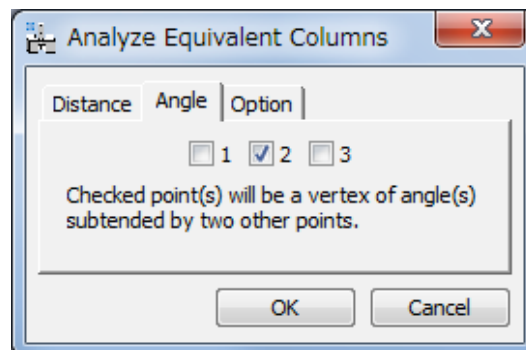| Component	Description
Save	Saves (with dialog) all images in a project of the same type as the front most image (e.g. strain map images).
Close	Closes (without saving) all images of the same type as the front most image.

Analyze Equivalent Columns Dialog

The user will have the option to decide the distances and/or angles to be evaluated.
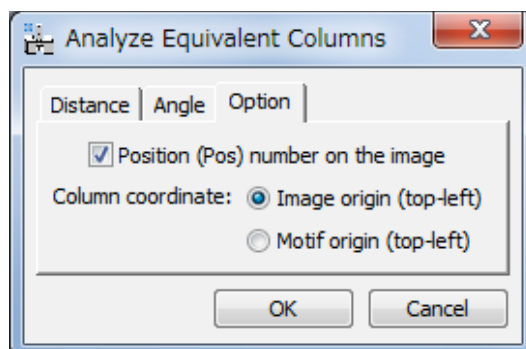
Distance Tab
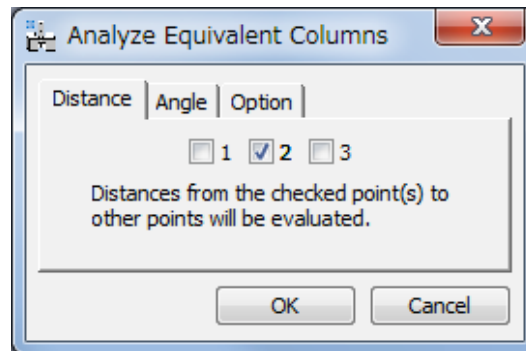
The number of each check box corresponds to the assigned number to the mouse click. All the distance(s) from the checked point to other points will be calculated.

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.

Show/Hide Sub-Menu

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

Create Vector Map Dialog

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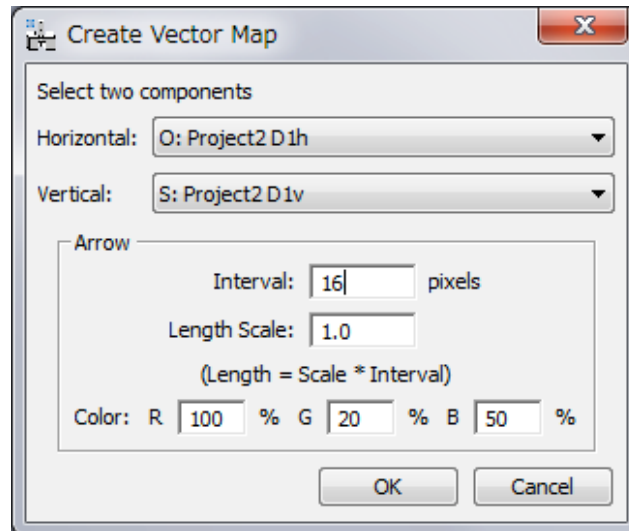
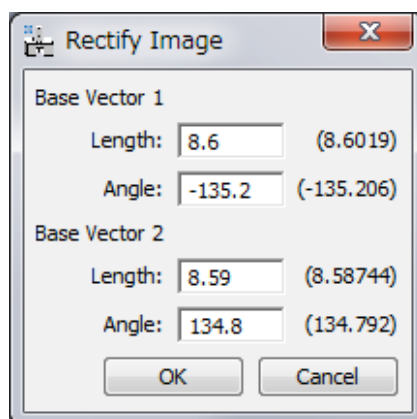| Component	Description
Horizontal	Select an image corresponding to the horizontal component.
Vertical	Select an image corresponding to the vertical component.
Interval	Specifies an interval to draw arrows (in pixel)
Length Scale	Specifies an arrow length. An actual length is Interval * Scale (in pixel)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

Distortion Correction Sub-Menu

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