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qDPC *for DigitalMicrograph*

*Quantitative Differential Phase Contrast
for STEM*

qDPC Manual 1.4 with 4D-STEM Module and Segmented Detector Module

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1. Introduction

The qDPC (quantitative Differential Phase Contrast) is a plug-in for use in Gatan's DigitalMicrograph for GMS 2.x and GMS 3.x. However, we will recommend you to use the latest GMS.

This qDPC manual is written to provide information on the basic functions of the qDPC plug-in, a procedure for installation of the Plug-In, some general tips on operation. This Guide assumes the user is familiar with image manipulation using DigitalMicrograph as well as Windows operating system.

The DPC calculates the phase distribution by integrating the DPC (Differential Phase Contrast) signals.

The 4D-STEM module generates the DPC signals from 4D-STEM data. The obtained DPC signals can be processed by the qDPC to calculate the phase distribution. There are two versions of the 4D-STEM module, namely 4DCanvas module and STEMx module.

In addition, the Segment Detector module can handle the DPC signal and calculate the phase distribution in real-time.

Technical Support

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2. *Installation*

This chapter describes hardware and software requirements to run the qDPC plug-in and an installation procedure of the plug-in.

2.1 Requirements

The qDPC plug-in runs under DigitalMicrograph environment, and the software and hardware requirements are similar to those for DigitalMicrograph itself.

2.1.1 Hardware requirement

The qDPC is commercial software and thus requires a license key (a USB dongle).

2.1.2 Software requirement

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

- **DigitalMicrograph.**
- **USB Key Driver**

2.2 Software Installation

The following modules should be installed. Please consult the ReadMe file for installation. The following modules should be placed in the folder “PlugIns” under “Gatan” folder at ProgramData.

- **qDPC Plug-in (.gtk and .dll)**
- **IPU Plug-in (Free-ware available at www.hremresearch.com)**
- **USB Key Driver**

Note: The PlugIns folder should exist under a normal installation of the DigitalMicrograph.

Installing qDPC Plug-in

qDPC plug-in (.gtk and .dll) can be installed by drag-and-drop copy to the folder “PlugIns” under “Gatan” folder at ProgramData.

Installing IPU Plug-in

IPU plug-in is a free plug-in. Please download the plug-in from the Scripts/Plugins page of HREM home page and install it according to the ReadMe file.

When the DigitalMicrograph is launched after placing the plug-ins the PlugIns folder, the menus “qDPC” and “IPU” will be appeared on the menu bar.

Installing Key Driver

The user key driver should be installed by following the instructions that comes with the key driver installer. You can find the key driver on our web site.

Additional modules

The qDPC plug-in has some modules for a 4D-STEM detector and a segmented detector. The additional modules can be installed by drag-and-drop copy to the in the same way as the qDPC plug-in.

NOTE: The additional module requires a separate license in addition to the qDPC license.

3. Getting Started...

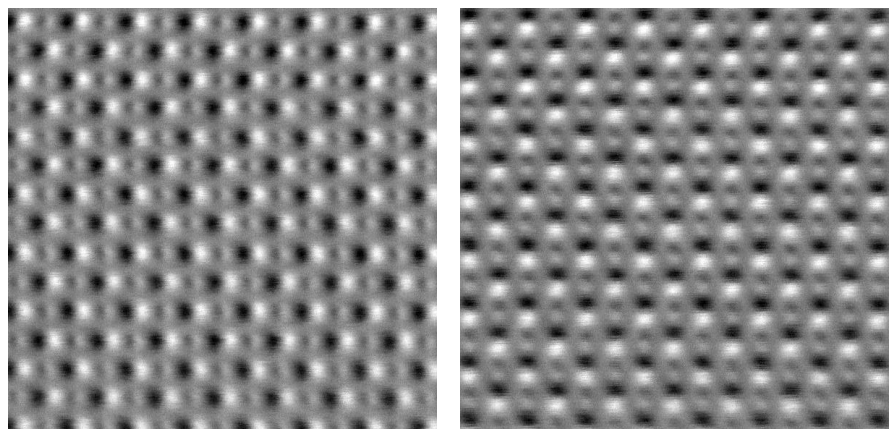
Using the qDPC plug-in is very simple. All the operations are menu driven, and process the front-most *active* image. This chapter briefly explains each command.

3.0 Essentials

3.0.1 What is DPC for STEM

DPC stands for Differential Phase Contrast, which is an imaging method for STEM to observe a phase object. In the original proposal by Dekkers and de Lang (Dekkers N. H. and de Lang H. Optik 41 (1974) 452), a set of semi-circular split detectors (see the next section) is assumed, and a signal is defined as a difference of outputs from the two detectors. Then, the signal shows an image similar to Differential Interference Contrast (DIC) in optical microscopy. Namely, we observe an image that comes from the relief of the surface under oblique illumination (see the DPC signals shown below from SrTiO₃). This contrast comes from the gradient of the phase distribution of the phase object.

It was shown later that the first moment of the diffraction distribution corresponds to the gradient of the phase distribution (Waddell E.M. and Chapman J.N. Optik 54 (1979) 83).



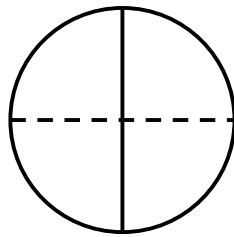
Two perpendicular DPC signals from SrTiO₃
(Data from Prof. Shibata, Tokyo Univ.)

3.0.2 Detector Geometry

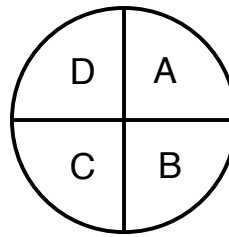
Since the first moment (center of mass, CoM) of the diffraction distribution corresponds to the gradient of the phase distribution, it is preferable to observe the whole diffraction pattern and calculate its CoM. However, since a quick acquisition of the diffraction pattern at each scanning position is a hard task, the DPC signal is normally acquired using the segment detector.

Segment Detector

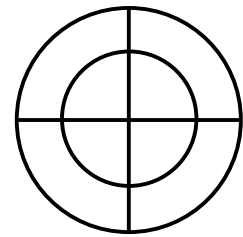
In the case of the segment detector the diffraction intensity over a section of the detector is integrated and the semi-circular split detector only acquires one component of the CoM vector perpendicular to the bisector. Therefore, a quadrant detector has commonly used at present. Using the quadrant detector we can generate two perpendicular split detector signals $((A+B)-(C+D))$ and $(A+D)-(B+C)$. However, in some cases the two differences of the opposite quadrants ($X=A-C$ and $Y=D-B$) are evaluated, and you will have two outputs. Even so, we can evaluate two split detector signals from $X-Y$ and $X+Y$, respectively.



Split Detector



Quadrant Detector



Double Quadrant Detector

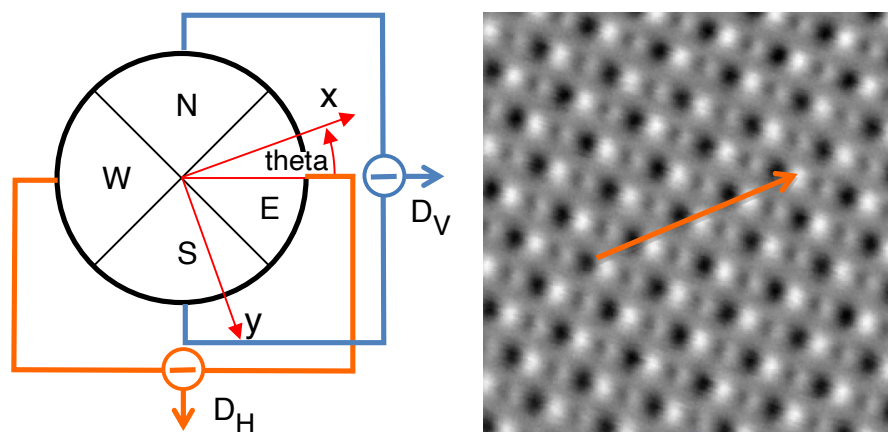
You may have a multi quadrant detector, for example, a double quadrant detector as shown in the right, or a single quadrant detector with a center hole. In the latter case, the detector is compatible with an EELS detector.

Pixel Detector

In order to calculate the first moment (center of mass, CoM) of the diffraction distribution we need to acquire the diffraction pattern at each scanning position. Since the dimension of the data is 4D (x, y, k_x, k_y) , this technique is called 4D-STEM.

3.0.3 Scan direction and the vertical direction of detector

Usually the direction of the detector is fixed (or not is adjusted for each acquisition), but the scan direction will be rotated to a preferred orientation of the sample by the operator for each acquisition. The detector output from almost separate atomic column consists of black and white as shown for SrTiO₃. However, when the scan direction differs from the detector orientation, the DPC signals will be shown in the image below.



It may be noted that the two outputs from the segment detector correspond to a two-dimensional vector with respect to the detector coordinate (orientation). Therefore, the DPC signals for the scanning direction will be rotated according to the vector algebra.

$$D_H = E - W$$

$$D_V = S - N$$

$$D_X = \cos(\theta) \times D_H - \sin(\theta) \times D_V$$

$$D_Y = \cos(\theta) \times D_V + \sin(\theta) \times D_H$$

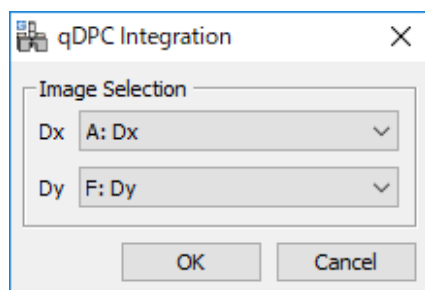
The vertical direction of the detector depends on the hardware and/or software designers. In the DPC we assume the vertical (y) direction is downward as commonly used in computer scientist. When the vertical direction of the detector of your system is upward, you can specify it using “Setup” command (see “Setup” command).

3.1 qDPC

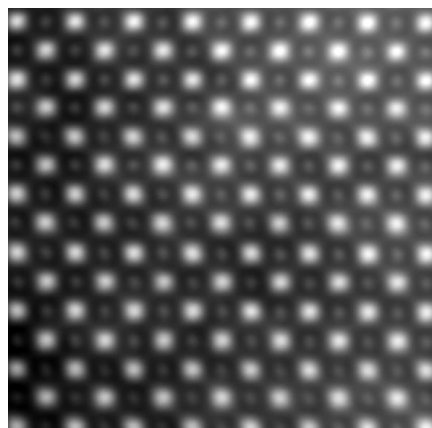


qDPC plug-in menu.

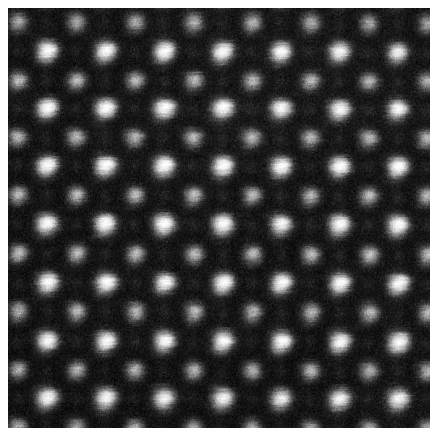
The most important part of this plug-in is a set of commands to retrieve the phase distribution from DPC signals. We strongly recommend using the integration based on DCT (Discrete Cosine Transform). When you have two DPC signals, you can calculate the object phase using one of the integration scheme by specifying these two signals from the opened image list:



Using the DCT command to the DPC signal for SrTiO_3 shown before, you can get the following phase distribution:



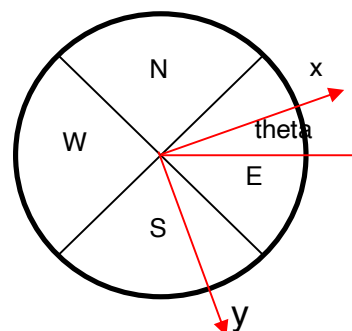
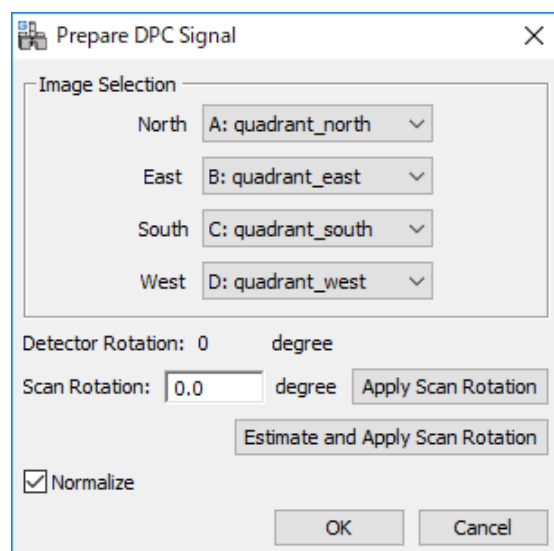
Retrieved Phase distribution



HAADF image

For comparison, the right image shows HAADF-STEM image acquired simultaneously. We can see oxygen atoms in the phase distribution obtained by DPC.

When you have four outputs from the segment detector, you can create the DPC signals using “Prepare DPC Signal” command:



Here, you can specify the direction of the fast scan. The DPC signals along the scan direction will be calculated from the four DPC outputs:

$$D_H = (\text{East}) - (\text{West}); D_V = (\text{North}) - (\text{South})$$

$$D_X = \cos(\text{theta}) \times D_H - \sin(\text{theta}) \times D_V$$

$$D_Y = \cos(\text{theta}) \times D_V + \sin(\text{theta}) \times D_H$$

When you press the “Apply Scan Rotation” button, the DPC signals will be rotated by the specified Scan Rotation angle, and the rotated DPC signals will be displayed in the new windows for your inspection.

If you don’t know the scan direction, you can use “Estimate Scan Rotation ” button. When you press this button, program tries to estimate the scan direction

using Detector Rotation angle, and show the estimated rotation angle in the input window.

If you check “Normalize,” the signal is normalized with the sum of the detector outputs.

4. Phase Retrieval

The first three integration commands for the DPC signals were introduced in the article: Ishizuka A, Oka M, Ishizuka I, Seki T and Shibata N: Microscopy **66**, 406 (2017).

4.1 DCT

The DPC signals are the derivative vector $(\partial\phi/\partial x, \partial\phi/\partial y)$ of the phase distribution $\phi(x, y)$. Therefore, we can calculate a Laplacian of the phase distribution ϕ from the DPC signals:

$$L(x, y) = \nabla^2 \phi(x, y) = \frac{\partial}{\partial x} \left(\frac{\partial}{\partial x} \phi(x, y) \right) + \frac{\partial}{\partial y} \left(\frac{\partial}{\partial y} \phi(x, y) \right)$$

Then, the phase distribution is obtained by solving this Poisson equation using DCT (Discrete Cosine Transform) with the Neumann boundary condition:

$$\begin{aligned} \phi(i, j) &= DCT^{-1} \left[\frac{DCT[L(i, j)](k, l)}{\lambda_k + \lambda_l} \right] \Delta^2 \\ &= DCT^{-1} \left[-\frac{DCT[L(i, j)](k, l)}{4 \sin^2(k\pi/2m) + 4 \sin^2(l\pi/2n)} \right] \Delta^2 \end{aligned}$$

Here, DCT and DCT^{-1} denote DCT and inverse DCT, respectively.

4.2 Extended FFT

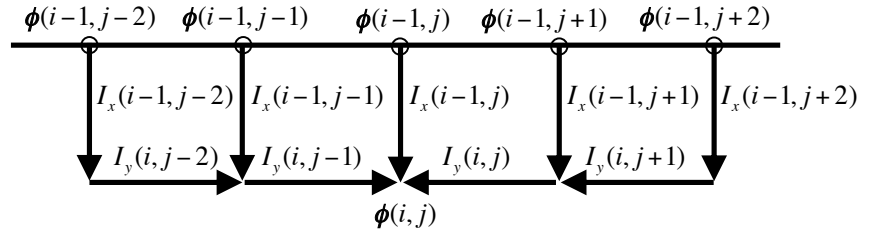
We can show the derivative of the symmetrically extended phase distribution $\phi_e(x, y)$ can be obtained from the observed DPC signal as follows:

$$\left\{ \begin{array}{l} \frac{\partial \phi_e}{\partial x} \approx \begin{bmatrix} I_x(x, y) & T_y[I_x(x, y)] \\ -T_x[I_x(x, y)] & -T_{xy}[I_x(x, y)] \end{bmatrix} \\ \frac{\partial \phi_e}{\partial y} \approx \begin{bmatrix} I_y(x, y) & -T_y[I_y(x, y)] \\ T_x[I_y(x, y)] & -T_{xy}[I_y(x, y)] \end{bmatrix} \end{array} \right\},$$

where I_x and I_y are the observed DPC signals, and T_x indicates a transpose of the data over the x-axis, and so on. Since the extended phase distribution $\phi_e(x, y)$ satisfies the periodic boundary condition, we can safely use FFT to solve the Poisson equation for $\phi_e(x, y)$.

4.3 Real-time integration

If there is no noise, any simple integration of the DPC signal that is the gradient of the phase distribution, will retrieve the object phase. However, the signal in the real world always contaminated by noise. Thus, we have developed a routine that estimates the phase value at $\phi(i, j)$ from multiple integration paths as shown below to average out the random noise.



If we can take the signal in real-time into DigitalMicrograph, we can use this integration scheme to show the phase distribution during progress of the scan, namely synchronized with the scan.

4.4 FFT1 and FFT2

Here, we have implemented two-reported phase retrieve routines using the FFT (Fast Fourier Transform). Please note that the results may have adverse effects when the sample does not satisfy periodic continuation at the image boundary, since the FFT implicitly assumes the periodic boundary condition. Therefore, we DON'T recommend to use these commands, but use them to check the expected artifacts.

FFT1:

$$\phi(x, y) = FT^{-1} \left[\frac{FT[I_x(x, y)](k_x, k_y) + iFT[I_y(x, y)](k_x, k_y)}{2\pi i(k_x + ik_y)} \right]$$

Close R, Chen Z, Sbibaba N and Findlay S.D: Ultramicroscopy **159**, 124 (2015)

FFT2:

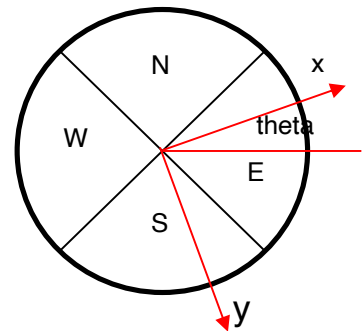
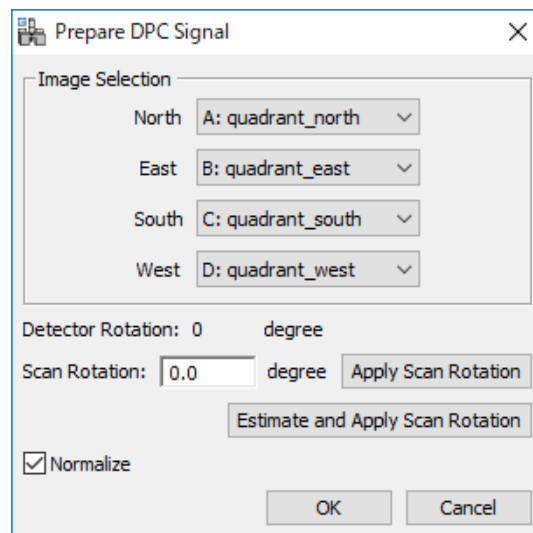
$$\phi(x, y) = FT^{-1} \left[\frac{k_x FT[I_x(x, y)](k_x, k_y) + k_y FT[I_y(x, y)](k_x, k_y)}{2\pi i(k_x^2 + k_y^2)} \right]$$

Lazic I, Bosch E.G.T and Lazar S: Ultramicroscopy **160**, 265 (2016)

5. Utilities

5.1 Prepare DPC signals

When you have four outputs from the segment detector, you can create the DPC signals using this command. You can select four signals from the opened image list for North, East, South and West signals, respectively.



Here, you can specify the direction of the fast scan in degrees. When you press the “Apply Scan Rotation” button, the DPC signals will be rotated by the specified Scan Rotation angle, and the rotated DPC signals will be displayed in the new windows for your inspection.

If you don’t know the scan direction, you can use “Estimate Scan Rotation” button. When you press this button, program tries to estimate the scan direction using Detector Rotation angle, and show the estimated rotation angle in the input window.

The DPC signals along the scan direction will be calculated from the four DPC outputs:

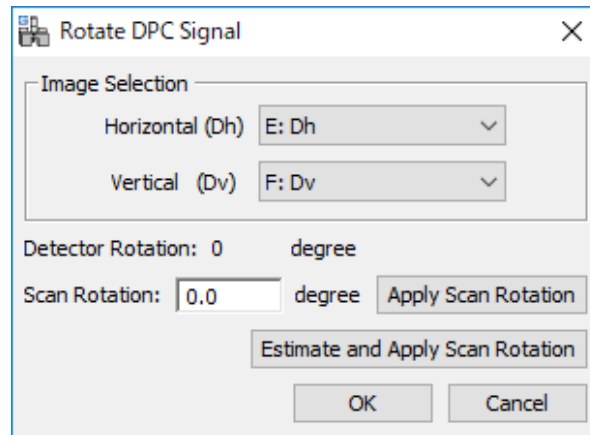
$$D_X = \cos(\theta) \times D_H - \sin(\theta) \times D_V$$
$$D_Y = \cos(\theta) \times D_V + \sin(\theta) \times D_H$$

where $D_H = E - W$, $D_V = S - N$

If you check “Normalize,” the signal is normalized with the sum of the detector outputs.

5.2 Rotate DPC signals

When you have the DPC signals (the CoM vector), but you want to rotate the vector according to the scan direction, you can use “Rotate DPC Signal” command:



Here, you can specify the direction of the fast scan in degrees. When you press the “Apply Scan Rotation” button, the DPC signals will be rotated by the specified Scan Rotation angle, and the rotated DPC signals will be displayed in the new windows for your inspection.

If you don’t know the scan direction, you can use “Estimate Scan Rotation” button. When you press this button, the scan direction estimated using Detector Rotation angle, and show the estimated rotation angle in the input window.

NOTE: When you don’t know the Detector Rotation angle, you can estimate it using the Estimate Detector Rotation command (see 5.4)

NOTE: If you want, you can directly assign the Detector Rotation angle in the Setup dialog (see 5.6 Setup command).

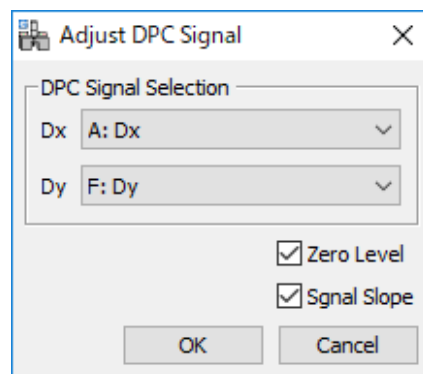
5.3 Adjust DPC signals

In the DPC experiment, you have to adjust the amplification factor of each segment, and then put the bright field disk at the center of the segment detector. This is a tedious procedure, and the adjusted conditions may not be kept during the whole experiment.

When the DPC signal(s) has a constant bias, the retrieved phase will have a slope in addition to the object phase distribution.

Furthermore, if the beam scan deflectors are not adjusted precisely, the bright field disk moves when the beam is scanned over the sample, and thus the DPC signal (the difference between the detectors) will increase or decrease with the beam scanning. This will give a slope on the DPC signals, and results in a (huge) parabola on the retrieved phase.

The command “Adjust DPC Signal” will balance the “Zero level” and/or remove the “Signal Slope” of the DPC signals. When there is a rectangle ROI on one of the DPC signals, the DPC signals are adjusted based on the signals within the ROI. Otherwise, the DPC signals are adjusted based on the whole area.



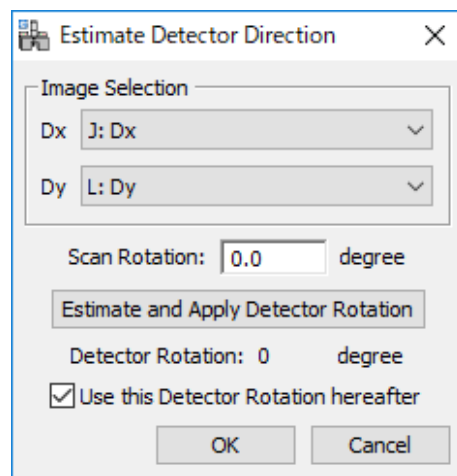
Please note that this command should be used very carefully. This is because this command will washout the sample feature, when there is a real slope due to the structure of your sample.

Nevertheless, using the ROI placed at a homogeneous area, you can adjust the DPC signals, even when there is, for example, an interface in the image.

5.4 Estimate Detector Rotation

The Detector Rotation angle is an angle of the detector with respect to the scan system. This command will estimate the Detector Rotation angle on the assumption that the specified Scan Rotation angle is correct.

If you know the scan direction when acquiring the DPC signals (the CoM vector) but you don't know the Detector Rotation angle, you can estimate the latter angle using this command. In this case, input the known scan rotation angle to the Scan Rotation field. The rotated DPC signals will be displayed in the new windows.



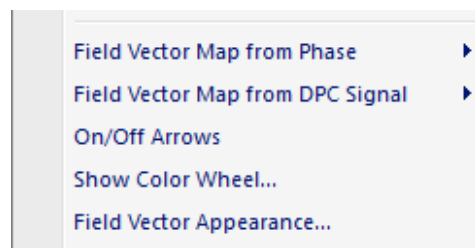
If the estimated vertical direction differs from the direction defined in the Setup dialog (see Section 5.6), you will get a warning message.

If you check “Use this Detector Rotation hereafter”, the value of Detector Rotation in the setup will be replaced by the estimated angle, and will be used in the subsequent DPC processing.

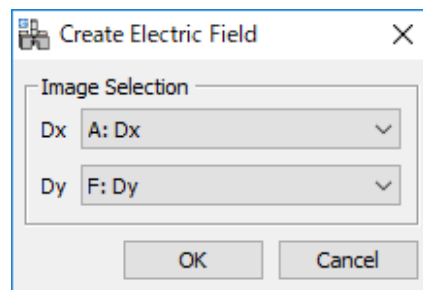
TIPS: Mostly, this command will be used for the DPC signals acquired with no scan rotation to estimate the Detector Rotation angle. However, you use this command for the DPC signals acquired with any Scan Rotation angle, provided you specify the correct Scan Rotation angle.

5.5 Field Vector Map

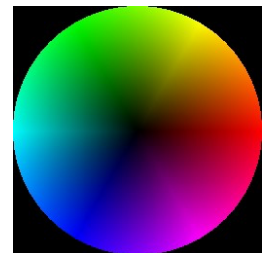
The DPC signals (CoM of the diffraction pattern) correspond to the gradient of the phase distribution, which is proportional to the projection of the electric scalar potential and/or magnetic vector potential along the beam direction. Thus, we can calculate electromagnetic field vector from the retrieved phase distribution. At first sight, this doesn't seem useful, because the observed DPC signals have simple relations to electromagnetic fields. However, we can calculate a smoother electromagnetic field from the retrieved phase than the observed DPC signals. This is because the gradient of the retrieved phase is less affected by noise than the DPC signals.



The field vector map can be calculated from the retrieved phase distribution (using “Field Vector Map from Phase”), or directly calculated from the two DPC signals (using “Field Vector Map from DPC Signal”). The former command will apply a front phase image, and the latter command requires two DPC signals selected in the dialog below:

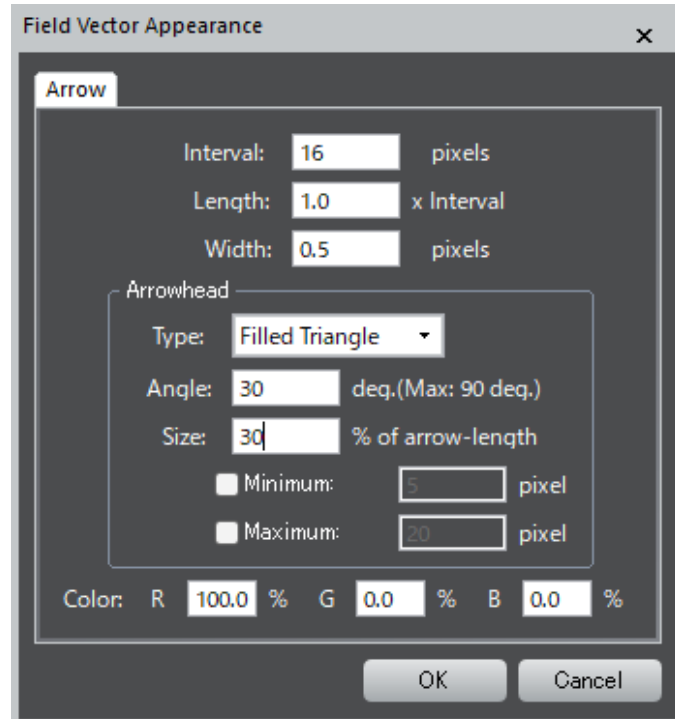


The direction and magnitude of the field vector is color coded defined by the color wheel, which can be displayed using “Show Color Wheel” command.

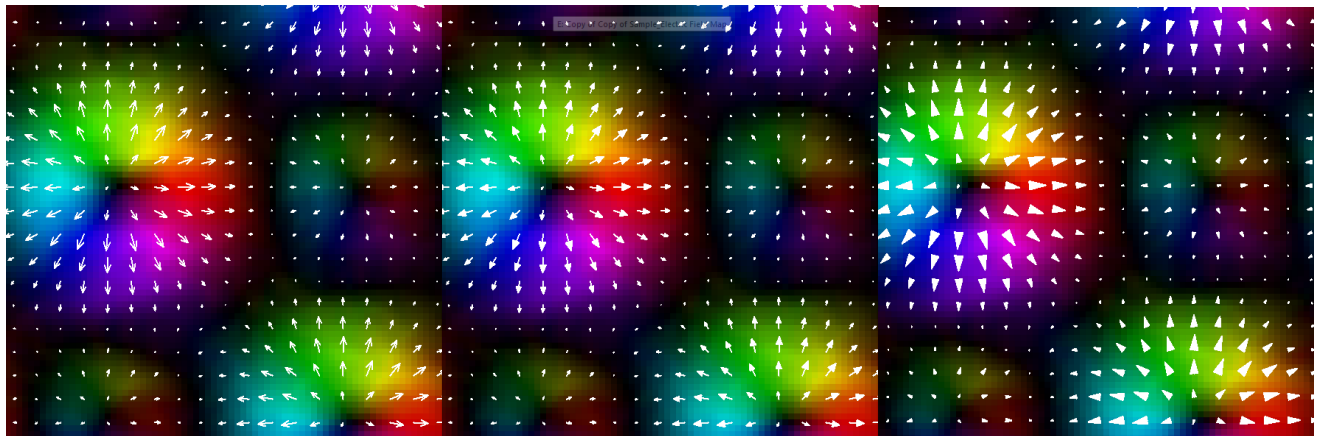


The direction and magnitude of the field vector can be indicated by the arrows, which you can show or hide using “On/Off Arrows” command.

Furthermore, you can change the spacing (interval) and the length of the arrows, as well as the color for the arrows using the “Field Vector Appearance” dialog shown below:



You can change also the Arrowhead type (Two Lines or Filled Triangle), arrowhead angle and length. (see Quick Reference Guide for details.)

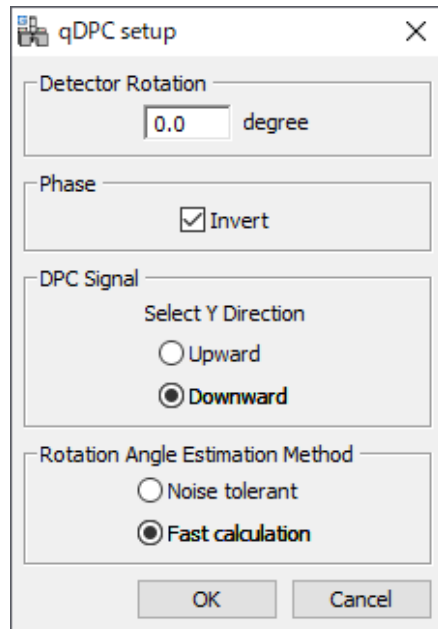


Two Lines

Filled Triangle

Filled Triangle (Size: 100%)

5.6 Setup



Detector Rotation: The detector angle with respect to the scan system is specified here. When you are not certain of the Detector Rotation angle, you can estimate it using Estimate Detector Rotation command.

Phase: The sign of the phase is somewhat arbitrary. Here, you can change the sign of the phase using “Invert” check box. The change of the display mode is sometimes useful to see the details of the image.

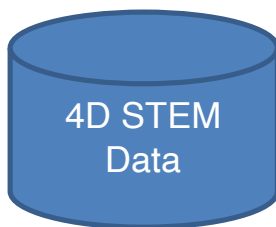
DPC Signal: The vertical direction of the detector depends on the hardware and/or software designers. In the DPC we assume the vertical (y) direction is downward as commonly used in computer scientist. Here, you can specify the vertical (y) direction of the detector of your system (upward or downward).

NOTE: If the estimated vertical direction differs from the direction defined in the Setup dialog, you will get a warning message.

Rotation Angle Estimation Method: There are two method to estimate the scan rotation angle. We recommend to use **Fast calculation**. However, if you have noisy images , you may want to use **Noise tolerant** method.

6. 4D-STEM Module

6.1 4D-STEM Data



The 4D-STEM data is a four-dimensional data $D(x,y,k_x,k_y)$, which is a set of the diffraction data obtained at each scanning position. Here, x and y correspond to a scan-position, and k_x and k_y represent the coordinate of the diffraction space. This kind of data becomes available by a rapid 2D detector, and a quick data transfer to the computer RAM.

From the 4D data we can calculate the first moment (center of mass, CoM) of each diffraction pattern and create the DPC signals.

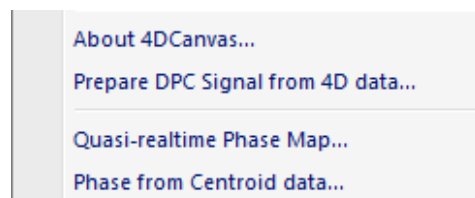
At this moment, the 4D-STEM modules for 4DCanvas (JEOL) and STEMx (Gatan) are available.

6.2 4DCanvas Module

The 4DCanvas module creates the DPC signals from the 4DCanvas data by calculating the CoM of the diffraction pattern. Using the DPC signals the phase map will be calculated by using the qDPC commands.

Furthermore, the 4DCanvas module calculates the phase map in quasi realtime just after the data acquisition from the COM data saved by 4DCanvas during the 4D-STEM data acquisition. In addition, the 4DCanvas module calculates off-line the phase map directly from the COM data saved by 4DCanvas.

The menu of the 4DCanvas module is shown below. Here, we have two groups of the commands, one for creating the DPC signals from the 4D-STEM data, and the two others for obtaining the phase map from the DPC signals in quasi realtime and off-line, respectively.



4Dcanvas module menu

6.2.1 Prepare DPC Signal from 4DCanvas

This command will calculate the CoM of 2D diffraction patterns and create the DPC signals. These DPC signals can be processed using qDPC commands.

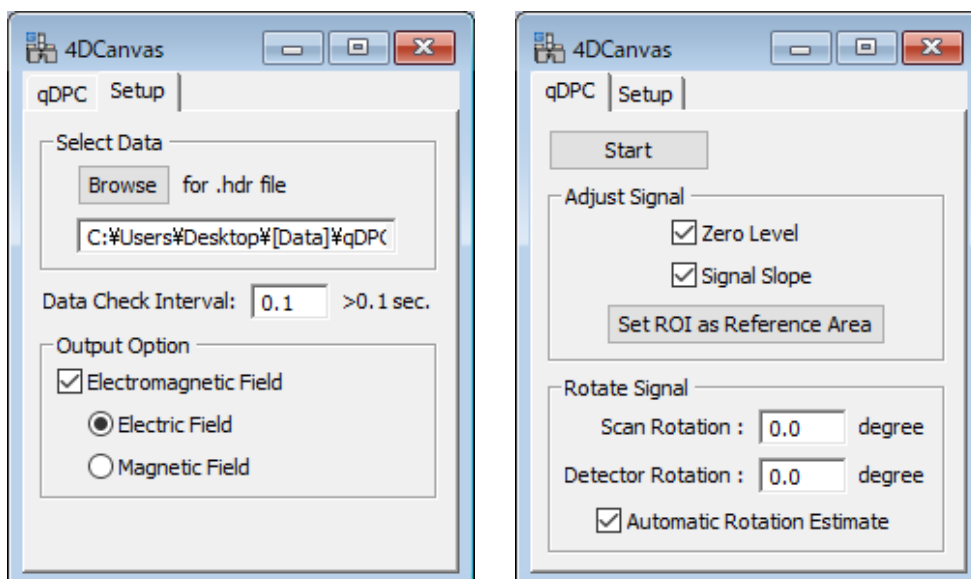
Selecting this command will open the dialog to select the data set. Here, please select a meta data file (.hdr), then two components of CoM will be calculated from the corresponding 4D data set, and displayed in the new windows.

6.2.2 Quasi-realtime Phase Map

This command will calculate a phase map from two centroid data (CoM) obtained by 4DCanvas. The phase map will be displayed in the new windows immediately just after each 4D-STEM data acquisition. The Phase map is calculated with the DCT (Discrete Cosine Transform) that is accurate for the DPC signal integration.

When we select this command, the dialog below with two tabs will be opened. Before obtaining the phase map in quasi-realtime, we have to specify the data set to be processed. To do so, select the Setup tab, and then click the browse button to choose a meta data file (.hdr) corresponding to the DPC signals (Centroid data: CoM) to be processed.

Here, you can specify an interval in sec to check a data update. The minimum check interval may be 0.1 sec. If you want, you can also calculate and display an electromagnetic field from the estimated phase map.



Then, go to the qDPC tab. The “Start” button will activate monitoring the DPC signals, and a phase map will be calculated just after each 4D-STEM data acquisition. This button changes to “Stop” that terminates the quasi-realtime phase calculation.

Here, there is the Adjust Signal pane, where you can choose phase calculation options: Zero Level and Signal Slope adjustments. You can specify the reference area to be used for these adjustments using “Set ROI as Reference Area”.

NOTE: A non-zero-average of the DPC signal will create a phase ramp in the phase map. On the other hand, a slope in the DPC signal will introduce a parabola (a quadratic surface) in the phase map.

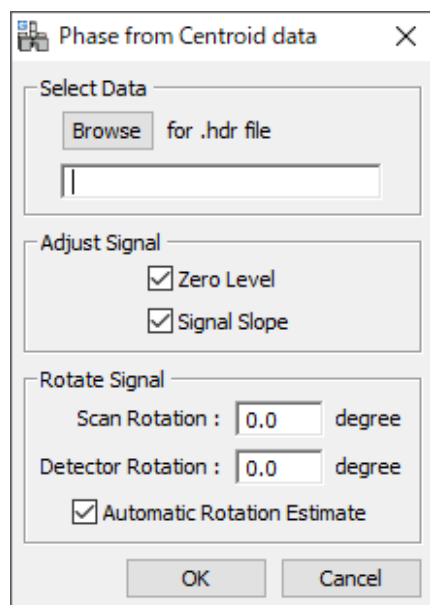
In the Rotated Signal pane, you can specify the Scan Direction (rotation angle). These values will be used to calculate the phase map. However, if you check the box for “Automatic Rotation Estimate”, the detector rotation angle is automatically determined from the observed DPC signals, and the determined scan direction will be used to calculate the phase map.

TIPS: Even after you stop the data acquisition, you can change the setting of the check box, or the text in the input field, or set the ROI. Then, a new phase image for the latest DPC signals will be calculated based on the new settings.

6.2.3 Phase from Centroid Data

This command will calculate a phase map directly from the DPC signals (Centroid; CoM) saved by 4DCanvas. The Phaser map is calculated with the DCT (Discrete Cosine Transform) that is accurate for the DPC signal integration.

When we select this command, the dialog below will be opened. Here, by clicking the browse button you can select a meta data file (.hdr) corresponding to the DPC signal (Centroid data) to be processed.



There is the Adjust Signal pane. Within this pane, you can choose phase calculation options: Zero Level and Signal Slope adjustments.

NOTE: A non-zero-average of the DPC signal will create a phase ramp in the phase map. On the other hand, a slope in the DPC signal will introduce a parabola (a quadratic surface) in the phase map.

TIPS: If you want to specify the reference area to be used Adjust Signal, please use the qDPC command (Adjust DPC signals) for the opened DPC signals.

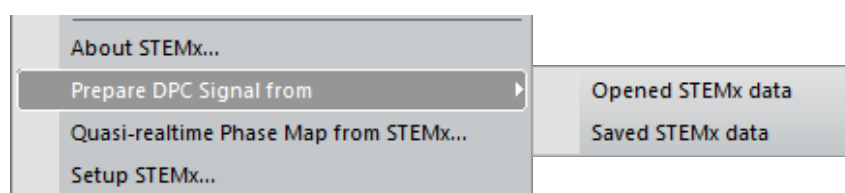
In the Rotated Signal pane, you can specify the Scan Direction (rotation angle). These values will be used to calculate the phase map. However, if you check the box for “Automatic Rotation Estimate”, the detector rotation angle is automatically determined from the observed DPC signals, and the determined scan direction will be used to calculate the phase map.

6.3 STEMx Module

The STEMx module creates the DPC signals from the 4D STEM data by calculating the CoM of the diffraction patterns. Using the DPC signals the phase map will be calculated by using the qDPC commands.

Furthermore, the STEMx module calculates the phase map from the COM data in quasi real-time just after the 4D-STEM data acquisition.

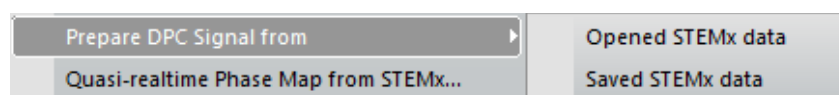
The menu of the STEMx module is shown below. Here, we have two commands, one for creating the DPC signals from the 4D-STEM data, and the others for obtaining the phase map from the DPC signals in quasi realtime.



STEMx module menu

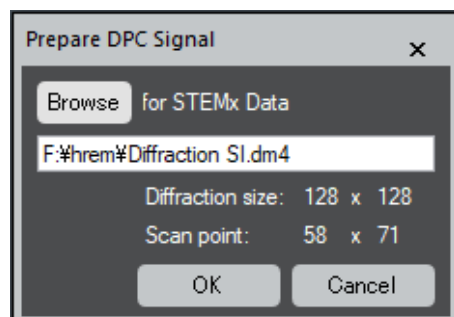
6.3.1 Prepare DPC Signal from (STEMx data)

This command will calculate the CoM of 2D diffraction patterns from the STEMx data, and create the DPC signals. There are two submenus, one for the opened STEMx data and the other for the STEMx data saved in the external mass storage:



You will get two DPC (CoM) signals displayed in new windows. The obtained DPC signals can be processed using the qDPC commands.

The submenu **Opened STEMx data** will be applied to the opened front-most STEMx data. On the other hand, the submenu **Saved STEMx data** will be applied to a STEMx data saved on an external memory device. Therefore, this command will open the dialog below to browse a STEMx file to be processed.

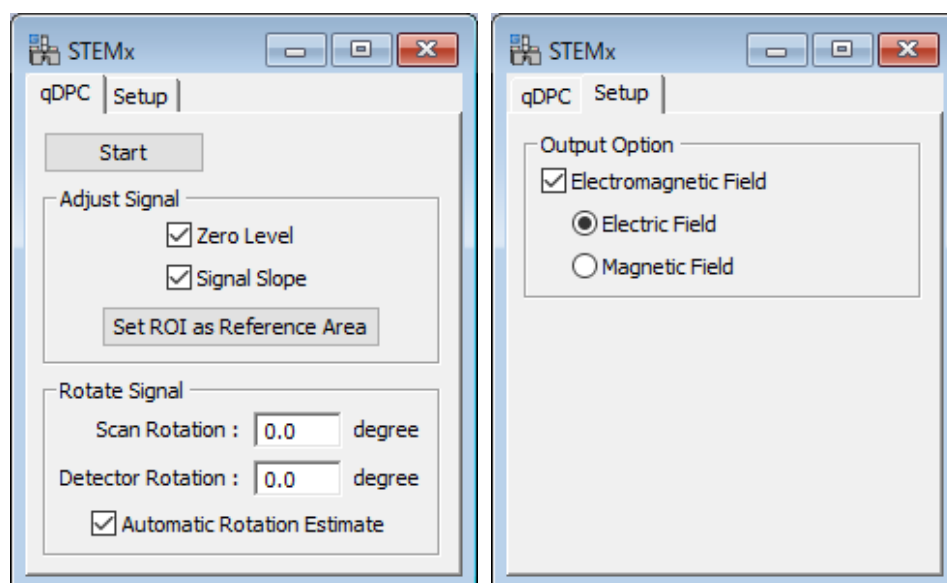


When the data is selected, the size of the diffraction patterns and the number of scanning points will be shown.

6.3.2 Quasi-realtime Phase Map from STEMx

This command will calculate a phase map in quasi-realtime from two centroid data (CoM) obtained from 4D-STEM data. The phase map will be displayed in the new windows immediately just after each 4D-STEM data acquisition. The Phase map is calculated with the DCT (Discrete Cosine Transform) that is accurate for the DPC signal integration.

When we select this command, the dialog below with two tabs will be opened.



The “Start” button will activate monitoring a new 4D-STEM data in the active workspace, and a phase map will be calculated just after a data acquisition. This button changes to “Stop” that terminates the quasi-realtime phase calculation.

Here, there is the Adjust Signal pane, where you can choose phase calculation options: Zero Level and Signal Slope adjustments. You can specify the reference area to be used for these adjustments using “Set ROI as Reference Area”.

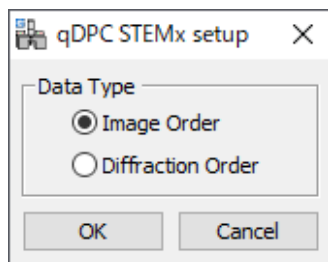
NOTE: A non-zero-average of the DPC signal will create a phase ramp in the phase map. On the other hand, a slope in the DPC signal will introduce a parabola (a quadratic surface) in the phase map.

In the Rotated Signal pane, you can specify the Scan Direction (rotation angle). These values will be used to calculate the phase map. However, if you check the box for “Automatic Rotation Estimate”, the detector rotation angle is automatically determined from the observed DPC signals, and the determined scan direction will be used to calculate the phase map.

TIPS: Even after you stop the data acquisition, you can change the setting of the check box, or the text in the input field, or set the ROI. Then, a new phase image for the 4D-STEM data in the active workspace will be calculated based on the new settings.

6.3.3 Setup STEMx

Now, the 4D-STEM data is saved in two ways: Image Order and Diffraction Order. In the former, the first two dimensions shows an image, while in the latter the first two dimensions shows a diffraction pattern. Thus, you have to select the data type in the Setup dialog shown below:



NOTE: When the image type of the 4D-STEM data is stores in the image tag, the program will read it automatically. Therefore, you don't need to specify the image type manually.

7. Segmented Detector Module

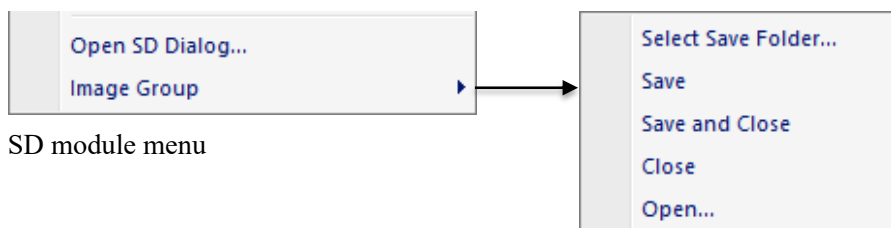
7.1 Real-time DPC signals from DigiScan II

The signals from a segmented detector can be acquired real-time using the DigiScan II (Gatan). The DigiScan II is commonly used to acquire the signals from the STEM detectors, say ADF (Annular Dark Field) and/or BF (Bright Field) detectors. Thus, one DigiScan II or two DigiScan IIs must be added to acquire four signals from a quadrant detector, or eight signals from an octant detector (double quadrant detector).

7.2 Segmented Detector (SD) Module

The Segmented Detector (SD) module calculates a phase distribution of the phase object in real-time from the DPC signals. Here, the DPC signals are obtained from the signals of the segmented detector that are acquired with the DigiScan II(s) synchronously with the progress of the scan.

The menu of the SD module is shown below. The first menu opens the main dialog to control the data acquisition and phase calculation. The other command is provided for the data management for the acquired images.



SD module menu

7.2.1 Open SD Dialog

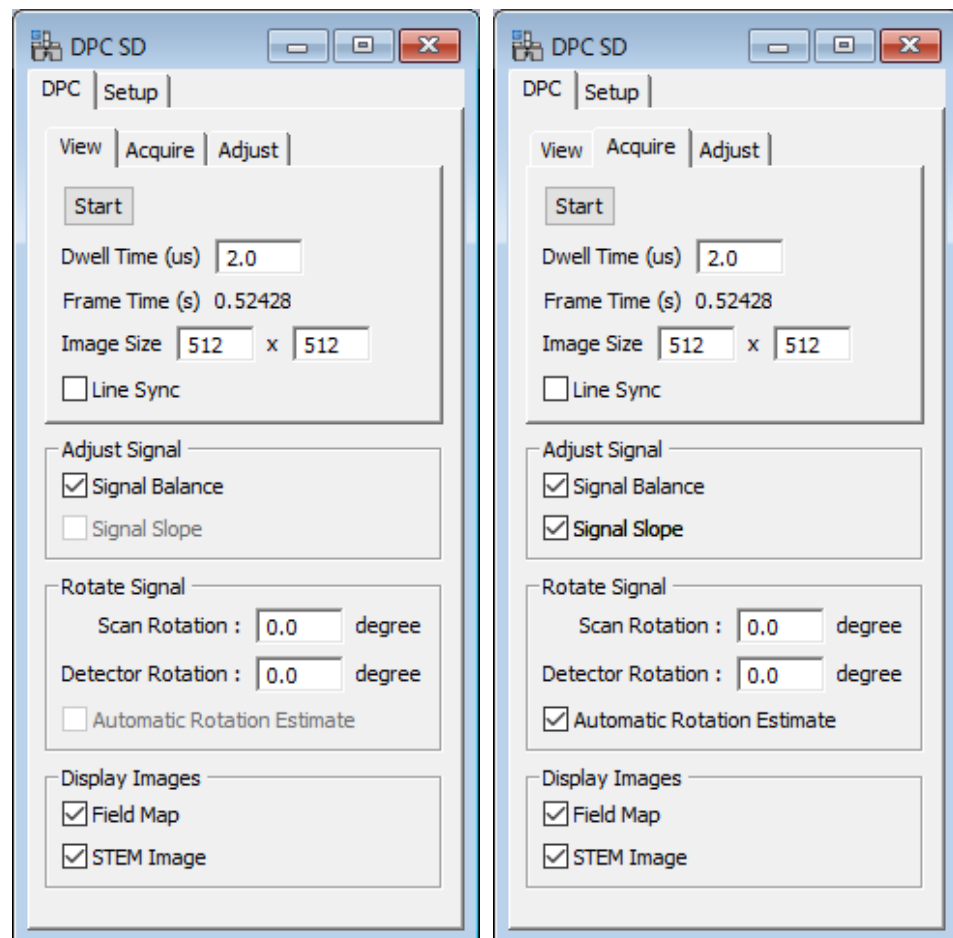
This command opens the dialog that has main two tabs, DPC and Setup, which are designed to control the data acquisition and data processing, and to set-up the parameters, respectively.

The DPC tab has three tabs: View, Acquire and Adjust tabs for each specific data acquisition and processing mode. The first two modes are used for data acquisition, and the last mode will be used by a service engineer.

View and Acquire Tabs

Here, you can specify the dwell time and the image size for each data acquisition mode.

In the View and Acquire mode, the phase map is calculated using the real-space real-time integration routine that is quick enough to synchronize with the progress of the scan. In the Acquire mode, the phase map is re-calculated just after data acquisition using the DCT (Discrete Cosine Transform) routine, which is an ideal integration method for the DPC signals.



There is the Adjust Signal pane. Here, you can choose phase calculation options: Zero Level and Signal Slope adjustments. In the View mode, the signal slope correction cannot be selected. In the Acquire mode, the signal slope adjustment will be done using the DCT routine after the data acquisition.

NOTE: A non-zero-average of the DPC signal will create a phase ramp in the phase map. On the other hand, a slope in the DPC signal will introduce a parabola (a quadratic surface) in the phase map.

In the Rotated Signal pane, you can specify the Scan Direction (rotation angle). These values will be used to calculate the phase map. However, if you check the box for “Automatic Rotation Estimate”, the detector rotation angle is automatically determined from the observed DPC signals, and the determined scan direction will be used to calculate the phase map. Please note that “Automatic Rotation Estimate” is not possible for the View mode.

TIPS: You can use the Acquire mode to take a high SNR DPC signals to calculate the phase map without software signal adjustment. Then, you can evaluate the detector adjustment. Furthermore, if there is electromagnetic disturbance that influences the scan precision, the scan instability may be detected from the phase map.

Setup Tab

Here, you can specify the Data Name that will be used when you save the data.

Currently, the DPC signals (CoM vector; DPCx and DPCy) will be estimated from a quadrant detector. When the segmented detector is an octant (a double quadrant), you have to choose the outer or inner quadrant.

The screenshot shows the 'DPC SD' dialog box with the 'Setup' tab selected. The dialog is divided into several sections:

- Data Name:** A text input field containing the word 'Project'.
- DPC Signal Segment:** Two radio buttons, 'Outer' (selected) and 'Inner'.
- Output Selection:**
 - Field Map:** Two radio buttons, 'Electric' (selected) and 'Magnetic'.
 - STEM Image:** Two radio buttons, 'BF (DPC SUM)' (selected) and 'ADF', followed by a text input field containing the number '8'.
- Signal Index:**
 - Data Depth:** A dropdown menu showing '4 byte'.
 - Outer:** A table with four rows: North (0), East (1), South (2), and West (3).
 - Inner:** A table with four rows: North (4), East (5), South (6), and West (7).

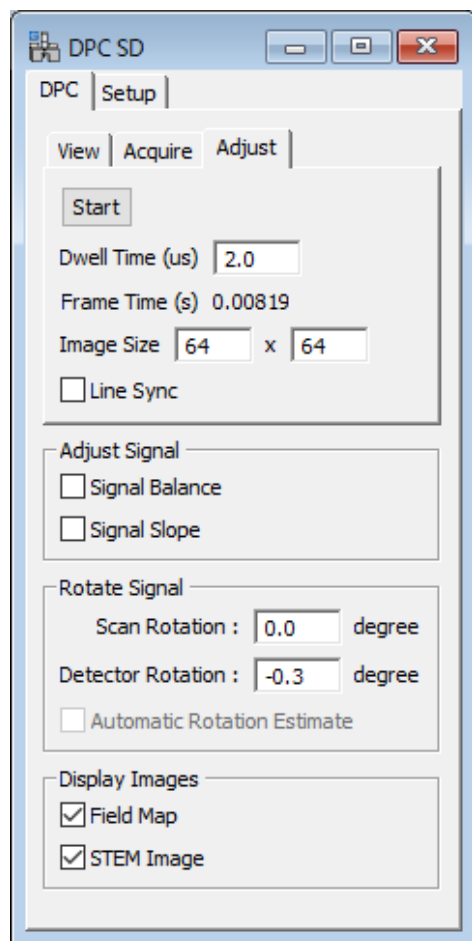
In the Output Selection pane, you can select the type of the field map, and the STEM image. The BF image will be calculated from the DPC signals. For the ADF image you have to specify the corresponding DigiScan signal index.

In the Signal Index pane, you have to specify the data depth of the DigiScan signal, and the DigiScan signal indexes for each segment of the detector. Please note the signal indexes depend on your setting of the DigiScan.

Adjust Tab

This tab will be used by a service engineer to adjust the segmented detector and the scan control. For this purpose, the DPC signals may be measured from a vacuum over a wide scan area.

Since the purpose of this mode is to adjust the experimental conditions, it is recommended to obtain the phase map as quickly as possible, say a several frames per second, using a small pixel numbers to cover a wide scan area.



NOTE: Contrary to other two modes, the phase map in this mode is calculated in quasi-realtime using the DCT (Discrete Cosine Transform) routine which is an ideal integration method for the DPC signals.

There is the Adjust Signal pane. However, both check boxes should be unchecked, if you want to examine the detector system adjustment. Nevertheless, you can evaluate the effect of software adjustment, when you check the box for the signal adjustment.

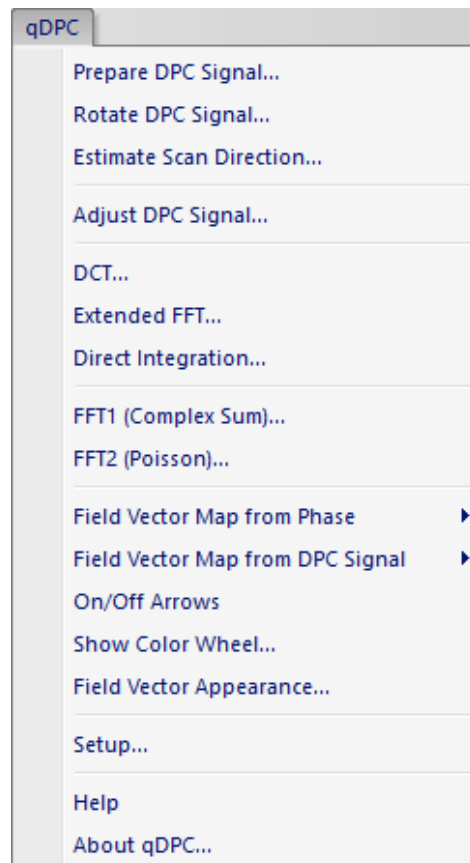
NOTE: A non-zero-average of the DPC signal will create a phase ramp in the phase map. On the other hand, a slope in the DPC signal will introduce a parabola (a quadratic surface) in the phase map.

In the Rotated Signal pane, you can specify the Scan Direction (rotation angle). These values will be used to calculate the phase map. Please note that “Automatic Rotation Estimate” is not possible for the Adjust mode.

The good values of the Detector Rotation should be determined by using a high SNR DPC signals with qDPC commands.

Quick Reference Guide

qDPC Main Menu



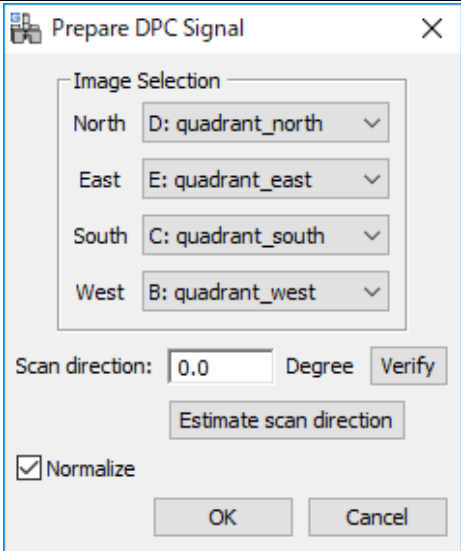
The commands in qDPC menu are described below.

Command	Description
Prepare qDPC Signals...	Calculates two components of DPC signal (CoM) using four outputs from a quadrant detector.
Rotate qDPC Signals...	Rotates the two observed DPC components relative to the detector.
Estimate Scan Direction...	Estimates a rotation angle of observed DPC components relative to the detector.
Adjust DPC Signals...	Adjusts the zero-levels and/or remove signal slopes from two DPC signals.
DCT...	Calculates a phase distribution from the DPC signal using DCT.
Extended FFT...	Calculates a phase distribution from the DPC signal using the extended FFT.

Direct Integration...	Calculates a phase distribution by directly integrating the DPC signal.
FFT1 (Complex Sum)...	Calculates a phase distribution using FFT from a complex sum of the DPC signals.
FFT2 (Poisson)...	Calculates a phase distribution using FFT of Poisson equation derived from the DPC signals.
Field Vector Map from Phase	Calculates a field vector map from the derivative of a phase distribution. Use this command when the front-most image is a calculated phase map.
Field Vector Map from DPC Signal	Calculates a field vector map simply from the observed DPC signals.
On/Off Arrows	Shows or hides arrows of the field vectors.
Show Color Wheel...	Shows a color wheel used for a field map.
Field Vector Appearance...	Changes the appearance of a field vector map.
Setup...	You can change some parameters depend on your system.

Prepare qDPC Signals Menu

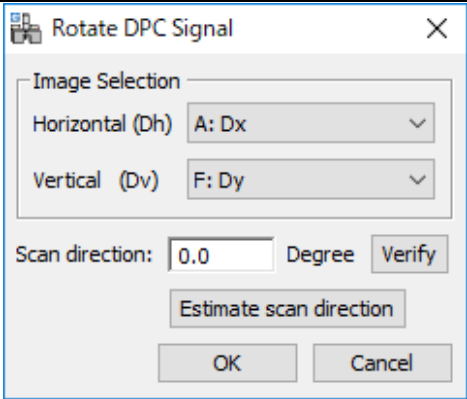
Calculates two components of DPC signal (CoM) using four outputs from a quadrant detector.

Dialog	
Component	Description
Image Selection	Select four signals (North/East/South/West) from the opened images.
Scan direction:	Rotation angle (in degree) of the horizontal DPC component relative to the detector. This is the sum of a deflector scan rotation angle and an angle of the

	deflector system relative to the detector.
[Verify]	When clicked, a new phase map will be calculated to check the rotation angle.
[Estimate scan direction]	When clicked, a scan direction will be estimated by assuming a commutative relation of derivatives (or an integrability).
Normalize	If checked, the DPC signals are normalized to unity.

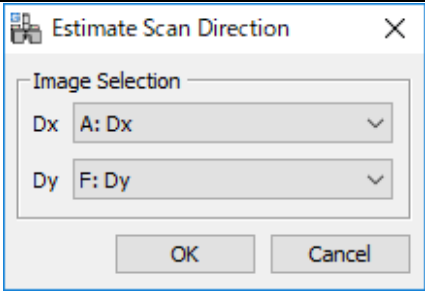
Rotate qDPC Signals Menu

Rotates the two observed DPC components relative to the detector.

Dialog	
Component	Description
Image Selection	Select two DPC signals from the opened images.
Scan direction:	Rotation angle (in degree) of the horizontal DPC component relative to the detector. This is the sum of a deflector scan rotation angle and an angle of the deflector system relative to the detector.
[Verify]	When clicked, a new phase map will be calculated to check the rotation angle.
[Estimate scan direction]	When clicked, a scan direction will be estimated by assuming a commutative relation of derivatives (or an integrability).

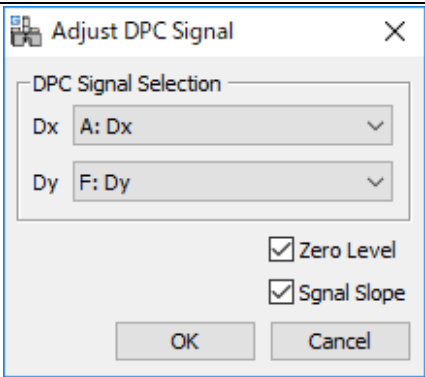
Estimate Scan Direction Menu

Estimates a rotation angle of observed DPC components relative to the detector.

Dialog	
Component	Description
Image Selection	Select two DPC signals from the opened images.

Adjust DPC Signals Menu

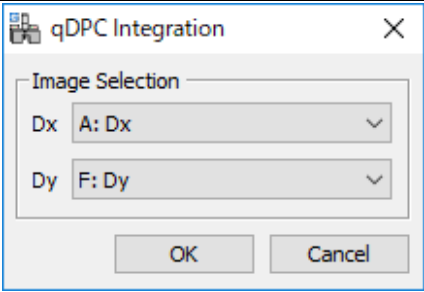
Adjusts the zero-levels and/or remove signal slopes from two DPC signals.

Dialog	
Component	Description
Image Selection	Select two DPC signals from the opened images.
Zero Level	If checked, the average of DPC signal is set to zero. If there is a rectangle ROI, the average is estimated over the ROI.
Signal Slope	If checked, the slope of DPC signal is subtracted from the signal. If there is a rectangle ROI, the slope is estimated over the ROI.

DCT/Extended FFT/Direct Integration/FFT1/FFT2 Menus

qDPC Integration Dialog

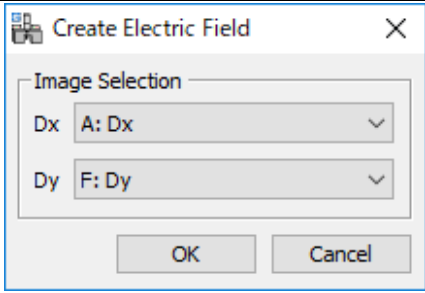
Calculates a phase distribution from the DPC signal using the selected method.

Dialog	
Component	Description
Image Selection	Select two DPC signals from the opened images.

Field Vector Map from DPC Signal Menu

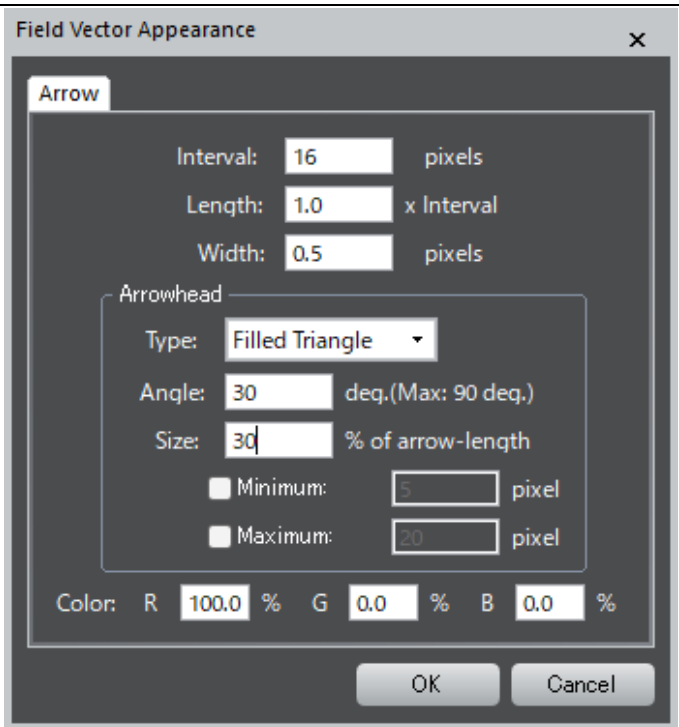
Create Electric/Magnetic Field Dialog

Calculates/displays a field vector map from the DPC signals.

Dialog	
Component	Description
Image Selection	Select two DPC signals from the opened images.

Field Vector Appearance Menu

Changes the appearance of a field vector map.

Dialog	
Component	Description
Interval	Specifies an interval to draw arrows (in pixel)
Length	Specifies an arrow length in terms of the Interval, namely an actual arrow length is determined by

	multiplying with Interval.
Width	Specifies a thickness of the arrow shaft and arrow lines (in pixel)
Arrowhead box	
Type	Arrow type selection from <i>Two Lines</i> and <i>Filled Triangle</i> .
Angle	Specifies a full angle of arrowhead (in degree).
Size	Specifies an arrowhead size as a fraction (%) of the total arrow shaft length. When this Size is set to 100%, a small arrowhead angle is preferable. If the size is set to 100%, the Minimum and Maximum settings will be disabled.
Minimum	If checked, the minimum arrowhead size (in pixel) will be set to this value. This setting prevents the arrows from becoming too small. When the arrow length itself becomes smaller than this minimum value, however, an arrowhead size will be set to the arrow length.
Maximum	If checked, the maximum arrowhead size (in pixel) will be set to this value. This setting prevents the arrows from becoming too large.
Color	Specifies an arrow color in RGB.