# qDPC
## for DigitalMicrograph

*Quantitative Differential Phase Contrast for STEM*

qDPC Manual 1.0
with 4D-STEM Module

# 1. Introduction

qDPC (quantitative Differential Phase Contract) is a plug-in for use in Gatan's DigitalMicrograph for GMS 2.x but works also with 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.

4D-STEM module calculates the DPC signals from 4D-STEM data, which can be processed by qDPC.

## Technical Support

General enquiries on the HREM-Filters should be sent to:

HREM Research Inc.
Email: support@hremresearch.com
Web: www. hremresearch.com

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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.

# 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-circler 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).
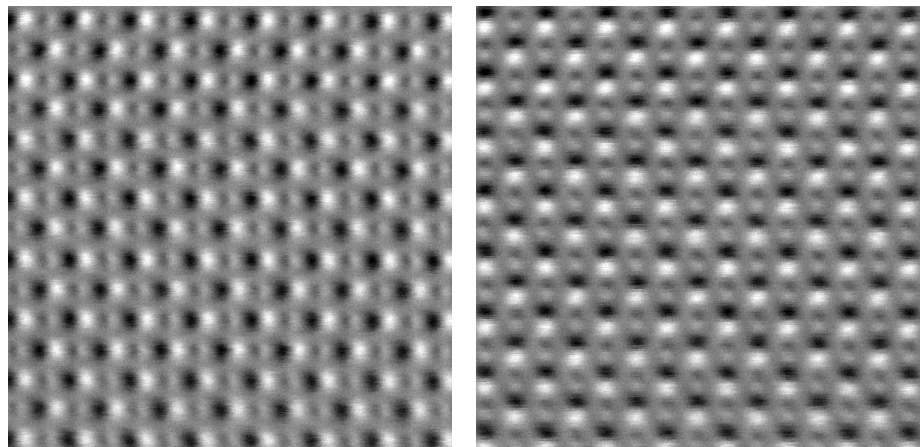


Two perpendicular DPC signals from SrTiO3
(Data from Prof. Shibata, Tokyo Univ.)

### 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.
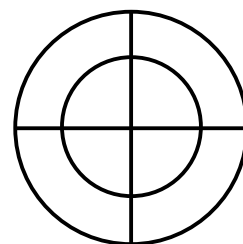
#### *Segment Detector*

In the case of the segment detector the diffraction intensity over a section of the detector is integrated and the semi-circler 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.
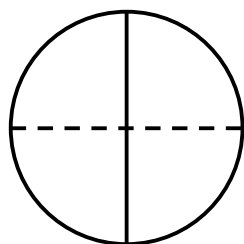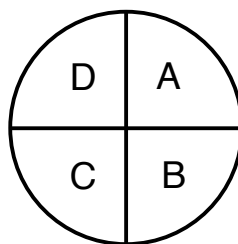


Split Detector          Quadrant Detector          Double Quadrant Detector

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.
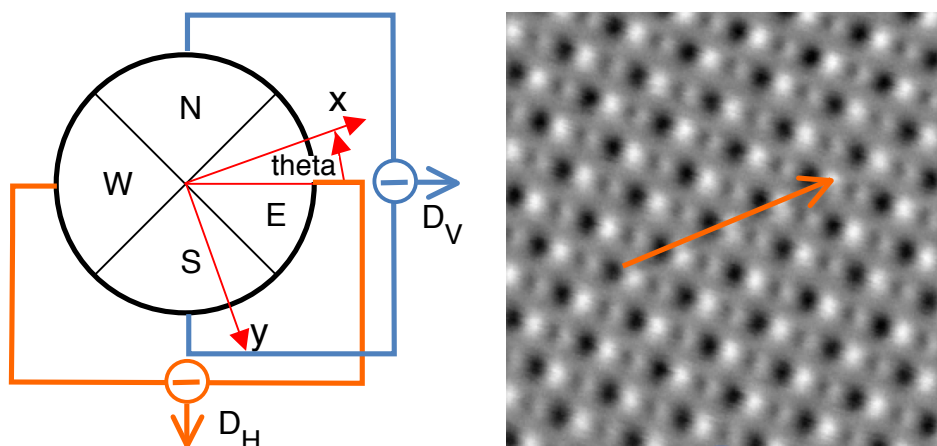


It may be noted that the two outputs from the segment detector correspond to a two-dimensional vector with respect to the detector coordinate (orientation). Therefore, the DPC signals for the scanning direction will be rotated according to the vector algebra.

$$D_H = E - W$$
$$D_V = S - N$$
$$D_X = \cos(theta) \times D_H - \sin(theta) \times D_V$$
$$D_Y = \cos(theta) \times D_V + \sin(theta) \times D_H$$

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
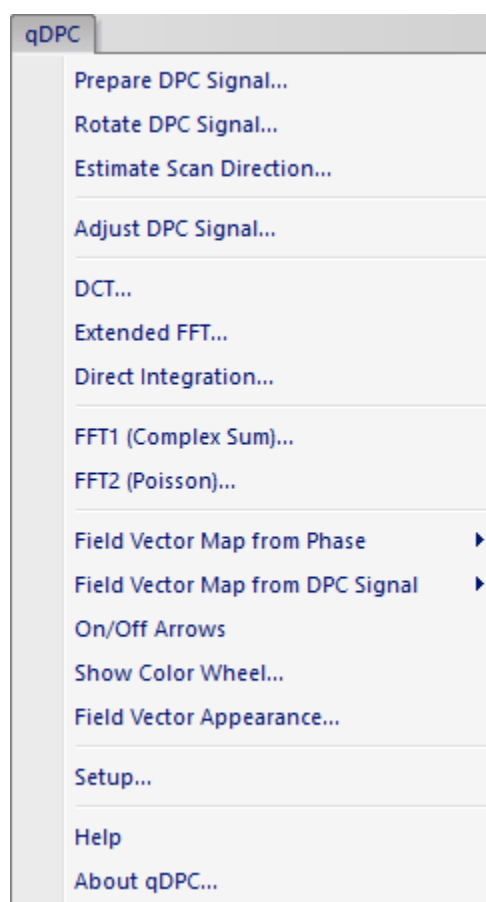


qDPC plug-in menu.

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:
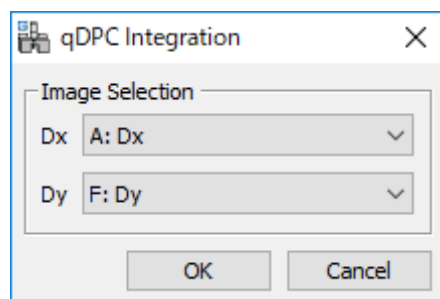


Using the DCT command to the DPC signal for $SrTiO_3$ shown before, you can get the following phase distribution:
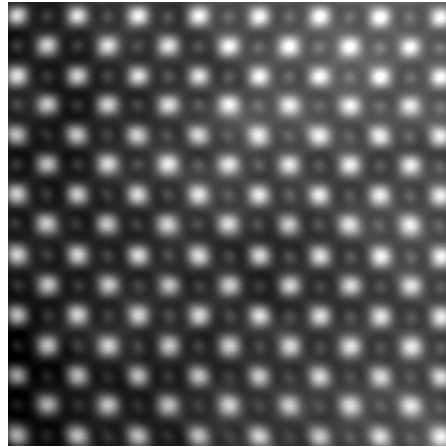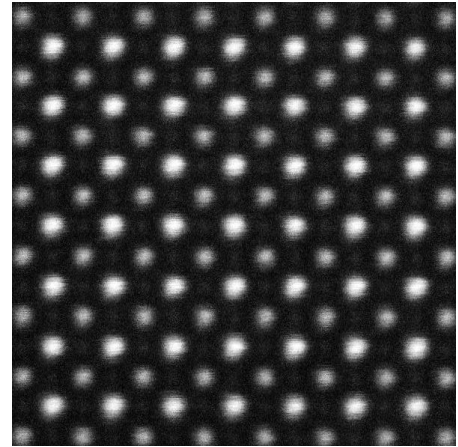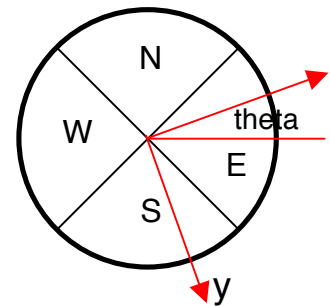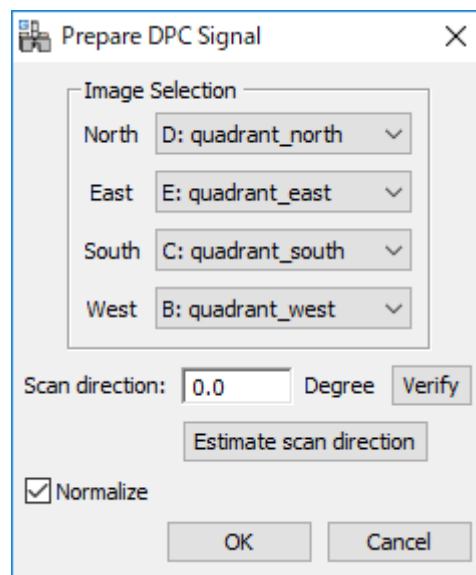
Retrieved Phase distribution HAADF image

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:

$$D_H = (East) - (West); D_V = (North) - (South)$$
$$D_X = \cos(theta) \times D_H - \sin(theta) \times D_V$$
$$D_Y = \cos(theta) \times D_V + \sin(theta) \times D_H$$

When you press "Verify" button, the rerated 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 direction" button. When you press this button, program tries to estimate the scan direction as well as the vertical direction of your system, 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

In the case of DPC signal, we observe the derivative vector ( $\partial\varphi/\partial x$, $\partial\varphi/\partial y$ ) of the solution $\varphi(x,y)$. Therefore, we can solve the Poisson equation using DCT (Discrete Cosine Transform) with the Neumann boundary condition:

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

Here, $L(i,j)$ is a Laplacian calculated from the DPC signals. $DCT$ and $DCT^{-1}$ denote DCT and inverse DCT, rexpectively.

## 4.2 Extended FFT

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

$$
\left\{
\begin{aligned}
\frac{\partial\varphi_e}{\partial x} &\approx \left[
\begin{array}{cc}
I_x(x,y) & T_y\big[I_x(x,y)\big] \\
-T_x\big[I_x(x,y)\big] & -T_{xy}\big[I_x(x,y)\big]
\end{array}
\right] \\
\frac{\partial\varphi_e}{\partial y} &\approx \left[
\begin{array}{cc}
I_y(x,y) & -T_y\big[I_y(x,y)\big] \\
T_x\big[I_y(x,y)\big] & -T_{xy}\big[I_y(x,y)\big]
\end{array}
\right]
\end{aligned}
\right. ,
$$

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 $\varphi_e(x,y)$ satisfies the periodic boundary condition, we can safely use FFT to solve the Poisson equation for $\varphi_e(x,y)$.

## 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.
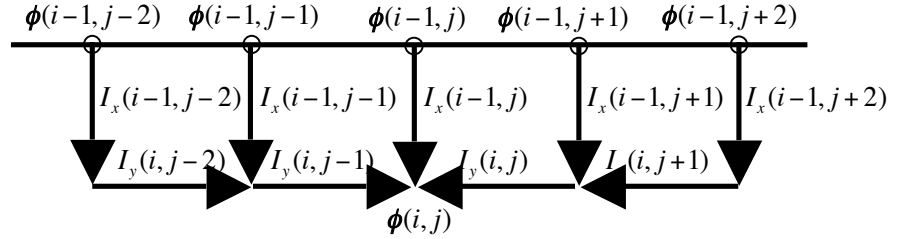


If we can take the signal in real time into DigitalMicrograph, we can use this integration scheme to show the phase distribution during progress of the scan, namely synchronized with the scan.

## 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:

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

Close R, Chen Z, Sbibata N and Findlay S.D: Utramicroscopy **159**, 124 (2015)
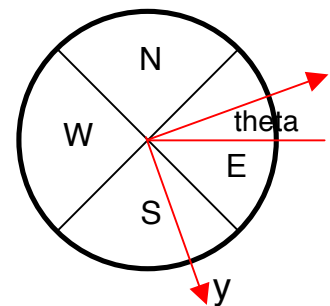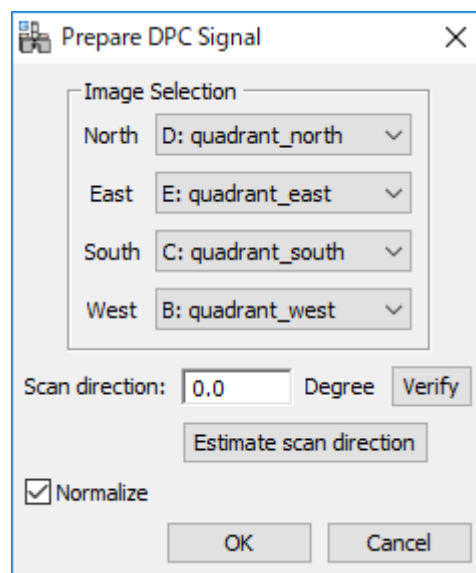
FFT2:

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

Lazic I, Bosch E.G.T and Lazar S: Utramicroscopy **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. If you don't know the scan direction, you can use "Estimate scan direction" button. When you press this button, program tries to estimate the scan direction as well as the vertical direction of your system, and show the estimated rotation angle in the input window.

When you press the "Verify" button, the DPC signals for the specified scan direction will be displayed in the new windows for your inspection.

The DPC signals along the scan direction will be calculated from the four DPC outputs:
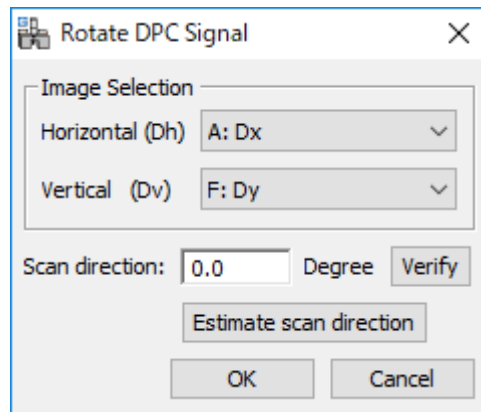
$$D_X = \cos(theta) \times D_H - \sin(theta) \times D_V$$
$$D_Y = \cos(theta) \times D_V + \sin(theta) \times D_H$$
$$\text{where } D_H = E - W, D_V = S - N$$

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. If you don't know the scan direction, you can use "Estimate scan direction" button. When you press this button, program tries to estimate the scan direction as well as the vertical direction of your system, and show the estimated rotation angle in the input window.

When you press the "Verify" button, the DPC signals for the specified scan direction will be displayed in the new image windows.

# 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 with in the ROI. Otherwise, the DPC signals are adjusted based on the whole area.
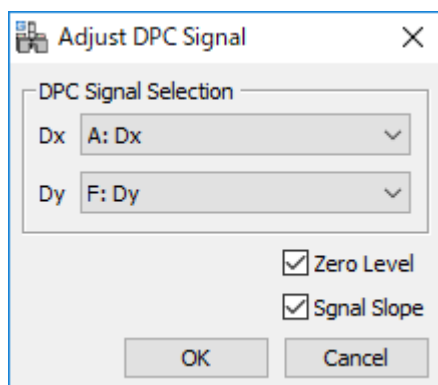
Please note that this command should be used very carefully. This is because this command will washout the sample feature, when there is a slope due to the structure of your sample.

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 Scan Direction

If you have not recorded the scan direction when acquiring the DPC signals (the CoM vector), you can estimate the scan direction as well as the vertical direction of your system using this command.
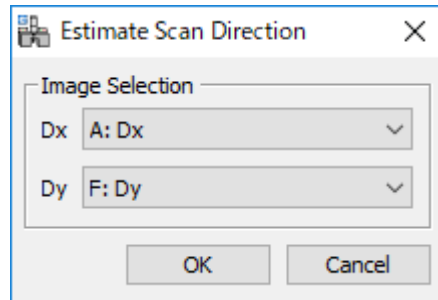


If the estimated vertical direction differs from the direction defined in the Setup dialog, you will get a warning message.

The rotated DPC signals will be displayed in the new windows.

## 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. This seems to be not rational, since the observed DPC signals have a simple relation to electromagnetic field. However, we can calculate a more smooth 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 then the DPC signals.
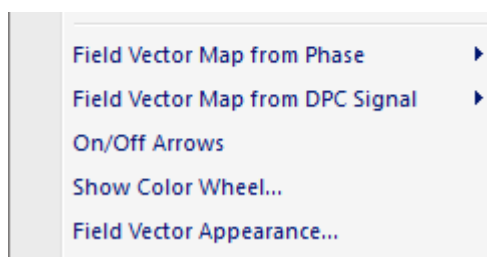


The field vector map can be calculated from the retrieved phase distribution (using "Field Vector Map from Phase"), or directly calculated from the two DPC signals (using "Field Vector Map from DPC Signals"). The former command will apply the front image, and two DPC signals should be selected for the latter command:
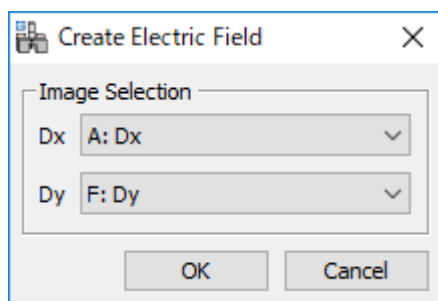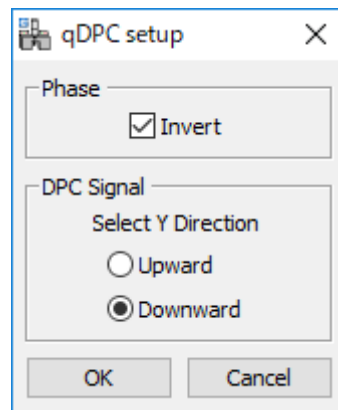


You can show or hide the arrows using "On/Off Arrows" command, and create the color wheel using "Show Color Wheel" command.



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:
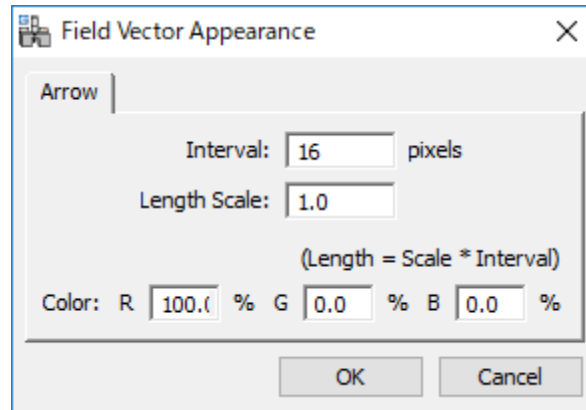
## 5.6 Setup



**Phase display mode**: The sign of the phase is somewhat arbitrary. Thus, 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.

**Vertical direction of the detector**: 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 in "Setup" dialog:

NOTE: When you are not certain of the vertical direction of your system, you can estimate using the command "Estimate Scan Direction." If the estimated vertical direction differs from the direction defined in the Setup dialog, you will get a warning message.

# *6. 4D-STEM Module*

## 6.1 4D-STEM Data
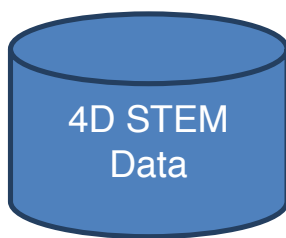
The 4D-STEM data is a four-dimensional data $D$(x,y,u,v), which is a set of the diffraction data obtained at each scanning position. Here, x and y correspond to a san-position, and u and v represent the coordinate of the diffraction space. This kind of data becomes available by a rapid 2D detector, and 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.

Now, the 4D-STEM modules for 4DCanvas (JEOL) and STEMx (Gatan) are avairable.

## 6.2 Prepare DPC Signal with 4D-STEM Module

The 4D-STEM module creates the DPC signals by calculating the CoM of the diffraction patter. Please consult the instruction about how to read the 4D-STEM data acquired by a specific camera/system.