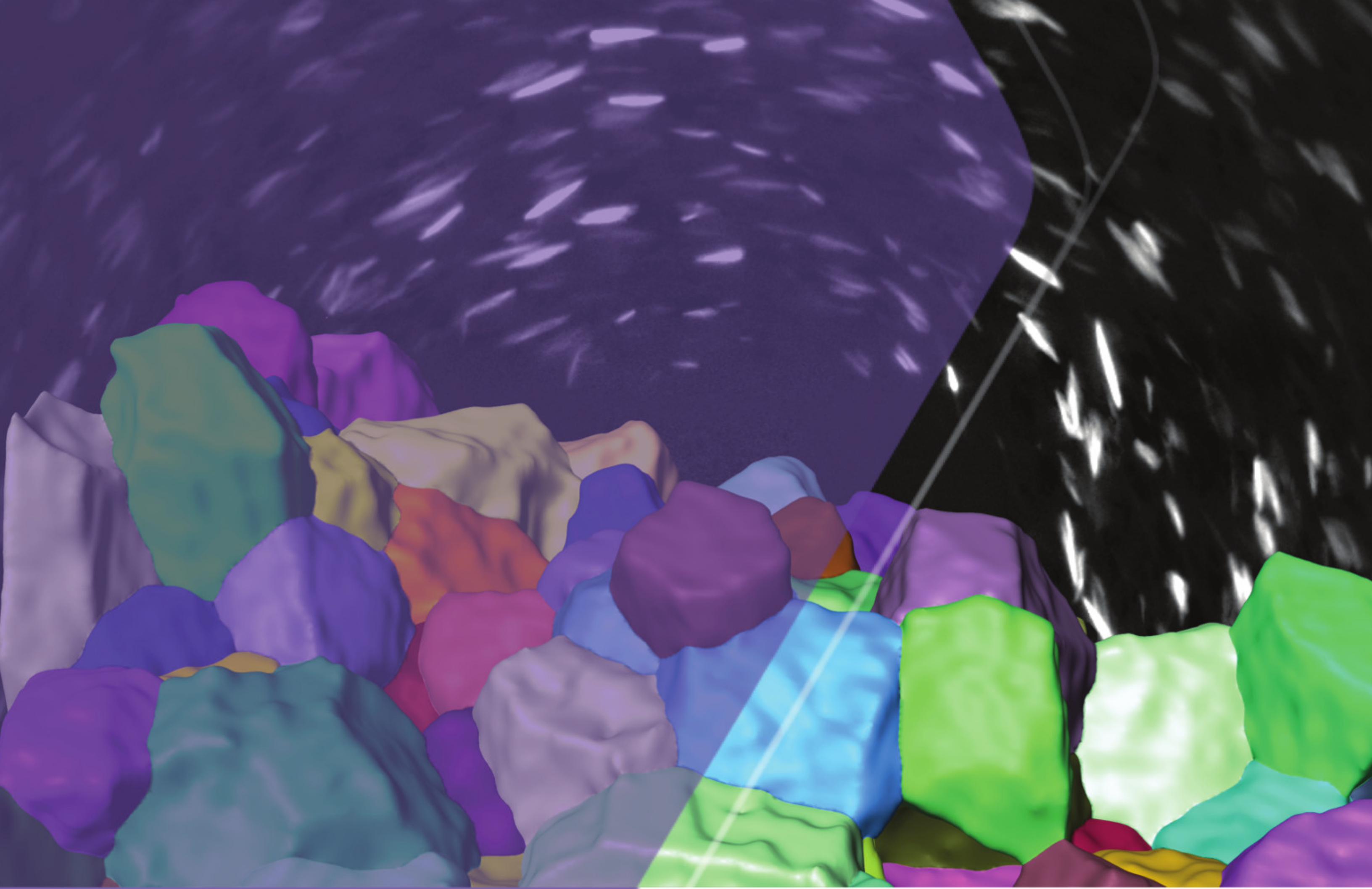

Release Notes

# GrainMapper3D™ 3.0

Non-destructive 3D Grain Mapping Solution for
Laboratory Diffraction Contrast Tomography

xnovotech

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# Contents

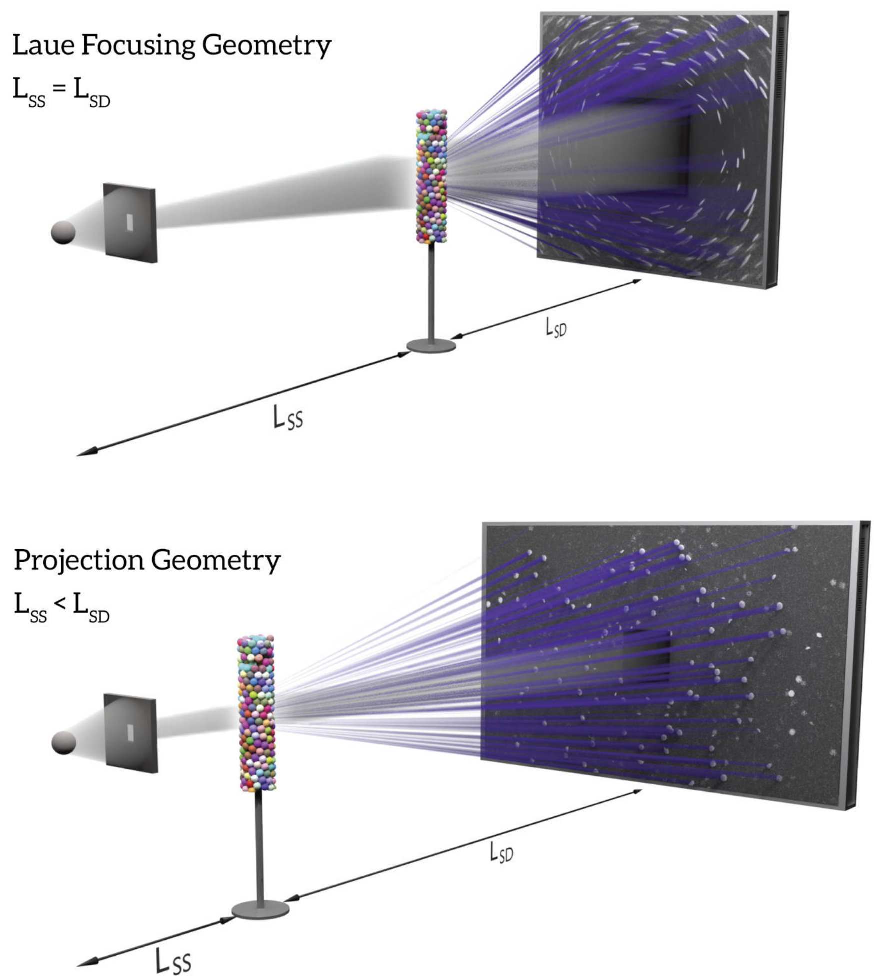
# New Features

## Projection Geometry Support

GrainMapper3D 3.0 introduces the reconstruction of Flat Panel data collected in projection geometry on the new crystallographic micro-computed tomography system ZEISS Xradia CrystalCT.

Figure 1 displays the geometry setup with example projections for the two supported data collection modes in Laue focusing and projection geometry using the corresponding detectors DCT4X and Flat Panel, respectively. Typical working distances are 12 mm < $L_{SS} = L_{SD}$ < 25 mm for Laue focusing geometry and 10 mm < $L_{SS}$ < 100 mm, 100 mm < $L_{SD}$ < 550 mm for projection geometry.

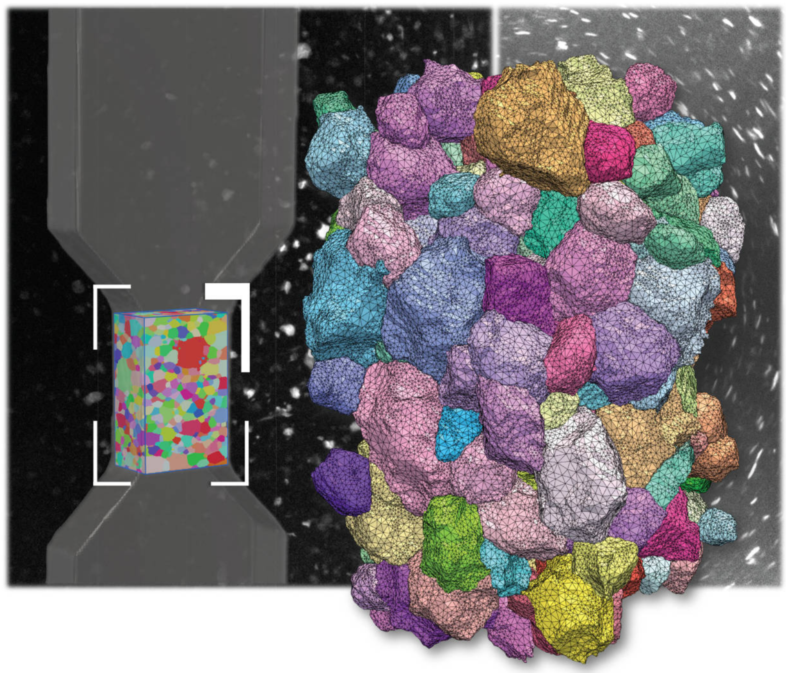
**Figure 1** LabDCT Setup for Laue Focusing and Projection Geometries



## Advanced Acquisition

Advanced Acquisition allows for seamless collection and subsequent reconstruction of DCT data for larger, irregularly shaped sample volumes as illustrated artistically in Figure 2. Setting up an advanced acquisition of DCT data is done using the new, dedicated DCT Acquisition Wizard, which is described in the next section.

**Figure 2** Advanced Acquisition for Large, Irregularly Shaped Specimens



While the *conventional* DCT scan performed using Scout-and-Scan is applicable when the *sample region of interest* (ROI) fits in the *beam field of view* (FOV), the DCT Acquisition Wizard allows for collecting DCT data with three new *advanced* acquisition strategies for samples where the ROI does not fit in the FOV.

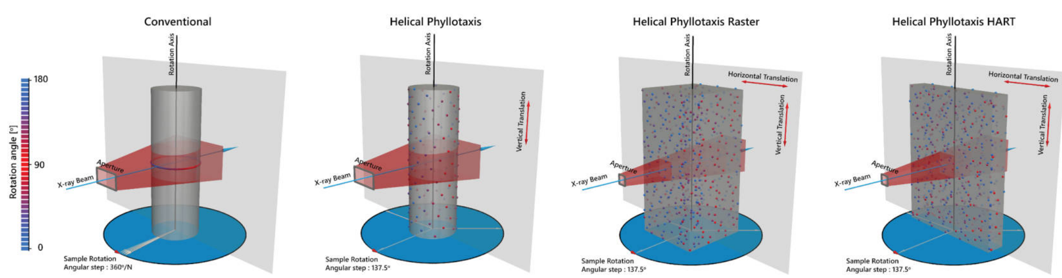
Depending on how the ROI exceeds the FOV one can choose between:

- *Helical Phyllotaxis* covers samples with a vertical extent larger than the beam height by means of a "Golden Angle" rotation of ~137.5° combined with a vertical translation of the order ~1–5 um between consecutive projections.
- *Helical Phyllotaxis Raster* is used if the ROI exceeds the FOV both vertically and horizontally. It combines the helical phyllotaxis rotation and vertical translation with a horizontal translation. The number of horizontal steps is the same for all projection angles.
- *Helical Phyllotaxis HART* (high aspect ratio tomography) is tailored for specimens with plate-like geometries. It combines the helical phyllotaxis rotation and vertical translation with a horizontal translation. The number of horizontal steps is adapted to tightly fit the ROI at every projection angle.

The advanced acquisition strategies are schematically compared to the conventional DCT scan in Figure 3. Here the points, colored by the sample rotation angle, mark where the center of the beam intersects the sample surface for individual projections.

**Figure 3** Advanced Acquisition Strategies for Different Specimen Shapes

| Scanning modes | Conventional | Helical Phyllotaxis | Helical Phyllotaxis Raster | Helical Phyllotaxis HART |
|---|---|---|---|---|
| FOV vs. ROI | ROI fits in FOV | ROI taller than FOV | ROI larger than FOV | ROI larger than FOV |
| Rotation stepping | 360°/N | 137.5° | 137.5° | 137.5° |
| Vertical translation | NO | YES | YES | YES |
| Horizontal translation | NO | NO | YES | YES - adaptive |




## DCT Acquisition Wizard

The **DCT Acquisition Wizard** is a new tool to help set up an advanced acquisition DCT scan. Only the principal structure and a few selected features of the DCT Acquisition Wizard will be outlined here.

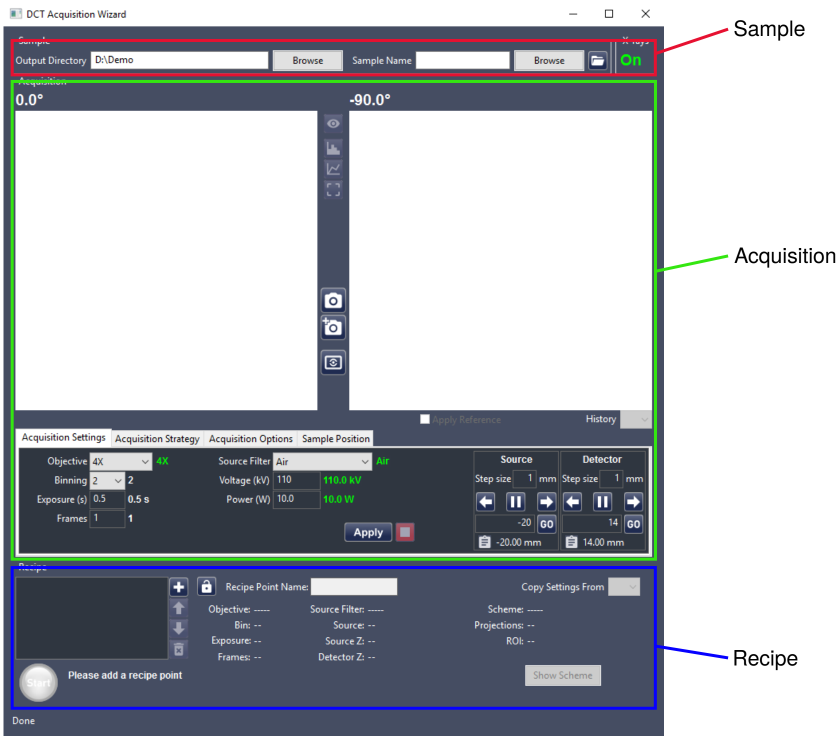
The reader is referred to the GrainMapper3D User’s Guide 3.0 for full instructions.

The DCT Acquisition Wizard is only to be installed on the acquisition workstation by ZEISS Service.

In order to perform an advanced acquisition of DCT data with the DCT Acquisition Wizard, select **Start > All Programs > Xnovo Technology ApS > Xnovo Acquisition Wizard** from the **Windows Start** menu. The **DCT Acquisition Wizard** window opens and requests the exclusive control over the Scout-and-Scan control system.

Figure 4 shows the layout of the DCT Acquisition Wizard, organized in **Sample** section, **Acquisition** section (including tabs for **Acquisition Settings**, **Acquisition Strategy**, **Acquisition Options**, and **Sample Position**), and **Recipe** section.

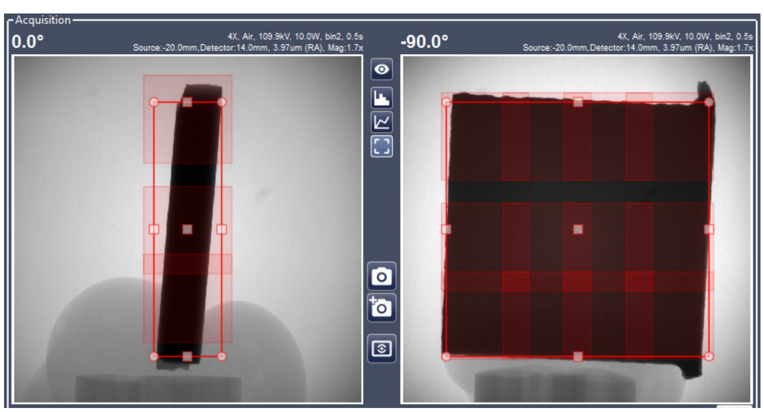
**Figure 4** Principal Layout of the DCT Acquisition Wizard




The *look and feel* of the DCT Acquisition Wizard is similar to Scout-and-Scan, and the user should be able to recognize many of the controls, for instance in the **Acquisition Settings**, **Sample Position** and **Recipe** sections.

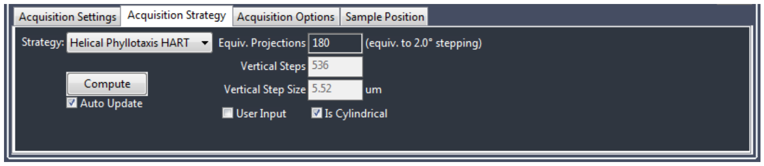
**Defining the ROI** is straightforward in the DCT Acquisition Wizard. Irrespective of the beam FOV, simply drag rectangles on top of the 0° and –90° absorption projections to cover the desired sample ROI as illustrated in Figure 5. The figure also shows the *FOV coverage* with respect to the ROI as the partly overlapping red boxes corresponding to the selected acquisition settings and strategy.

**Figure 5** Defining the ROI in the DCT Acquisition Wizard



The new *advanced* acquisition strategies outlined in Figure 3 can be selected in the **Strategy** drop-down of the Acquisition Strategy tab, see Figure 6.

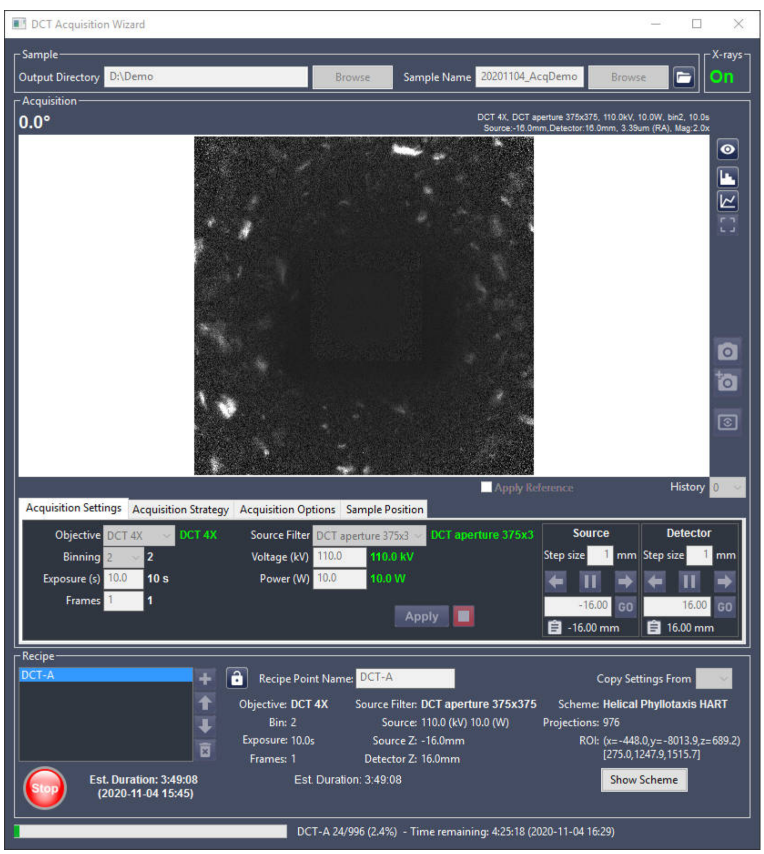
**Figure 6** Defining the Acquisition Strategy in the DCT Acquisition Wizard




The number of **Equivalent Projections** must be provided by the user based on the detector working distance. The scanning modes with Helical Phyllotaxis motion then fits this number of projections into the aperture FOV height by adjusting the **Vertical Step Size** between consecutive images accordingly. The number of **Vertical Steps** then follows to cover the entire height of the ROI defined by the user. Uncheck **Is Cylindrical** if applicable for the selected acquisition strategy and the sample has square or rectangular shape.

Figure 7 show the DCT Acquistion Wizard during a typical scan. The progressing scan views the latest projection in the Acquisition section, while the estimated time remaining is given next to the progress bar at the bottom.

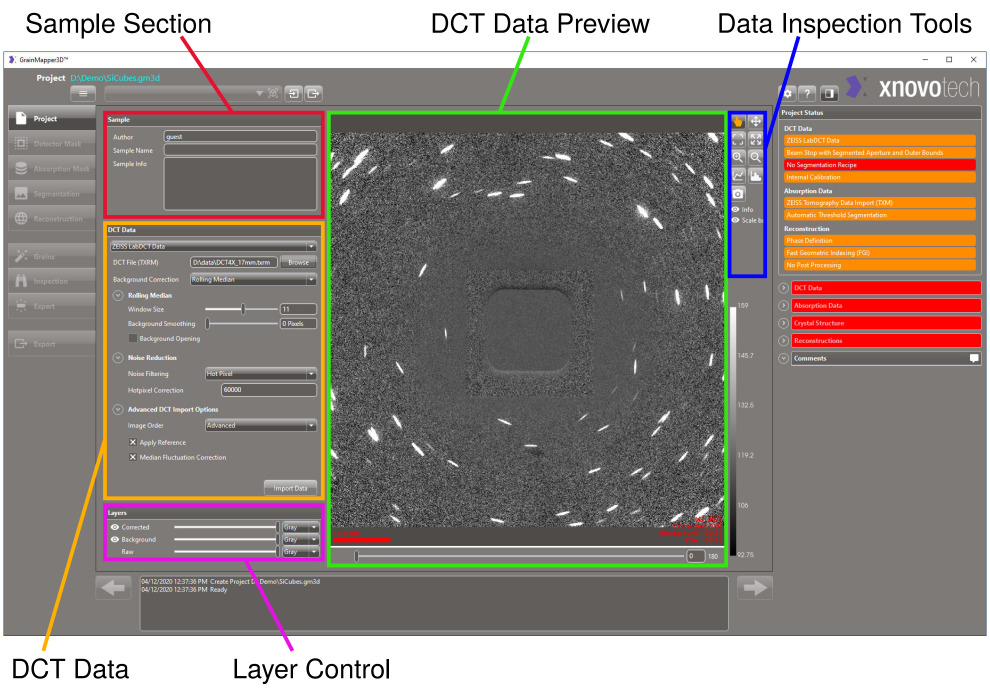
**Figure 7** DCT Scan in Progress in the DCT Acquisition Wizard



## DCT Data Import with Preview

The **Project** tab of GrainMapper3D has been redesigned to make space for a more sophisticated **DCT Data** import section with a live **DCT Data Preview.** The **Project** tab now focuses on the choice of appropriate DCT data import parameters to perform a better background correction with feedback. The absorption data import has been moved to the **Absorption Mask** tab. Figure 8 shows the redesigned **Project** tab for a new project organized in sections **Sample**, **DCT Data** and **Layers**. Parts of the former advanced DCT import options have been migrated into a new **Background Correction** group and **Noise Reduction** group.

**Figure 8** New Layout of Project Tab with DCT Data Import Preview




**Background Correction** The former DCT data import options has been moved into the **Rolling Median** background correction method and a new **Iterative Background** correction method has been added. Table 1 details the new controls for **Background Correction** of the Diffraction Contrast Patterns (DCPs).

**Noise Reduction** A new noise reduction method **Denoising** has been added. Table 2 gives an overview of the new controls for **Noise Reduction** of the DCPs. The noise reduction is performed on the raw DCPs after reference correction and prior to background calculation and subtraction.

**Advanced Acquisition Support** By default, the DCPs are resorted such that similar sample positions follow each other. Sorting is important for samples with a footprint larger than the beam stop, where sample attenuation contributes to the background pattern depending on both scan angle and sample position. Sometimes, mostly for helical phyllotaxis scans without horizontal sample translations, there are artifacts in the background that arise from the sample absorption and can be reduced by changing the **Image Order** to **Scan Order**, see Table 3.

**Layer Control** The visual appearance of the preview can be adjusted using the **Layer** control as described in Table 4. A cache for the DCT Data Import Preview allows quicker switching back and forth between already calculated import settings.

**Table 1** New Controls for DCT Background Correction in Project Tab

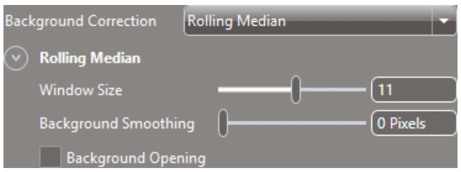
| Control | Function |
|---|---|
|  | **Rolling Median Background Correction** for **DCT Data:**<br>• **Window Size**, apply the rolling median correction over the specified number of successive images. Subtracts pixel-wise median of image stack.<br>• **Background Smoothing**, apply a 2D Gaussian filter to the rolling median background image with the specified sigma value (in pixels). Should only be used if no reference was collected.<br>• **Background Opening**, check to apply a morphological opening denoising step on the rolling median background image. |
|  | **Iterative Background Correction** for **DCT Data:**<br>• **Window Filter**, choose between:<br>– **Moving Average**, average over images in window**,**<br>– **Rolling Median**, take median over images in window, or<br>– **Gaussian**, images in window will be averaged with Gaussian weighting.<br>• **Window Size**, apply the above selected window filter over the specified number of images.<br>• **Iterations**, specify the number of adaptive background interpolation steps to be performed.<br>• **Sensitivity**, set intensity threshold over window average, above which intensity is replaced by interpolated value.<br>• **Sigma**, set Gaussian shape parameter for 2D smoothing at every iteration. |

**Table 2** New Controls for DCT Noise Reduction in Project Tab

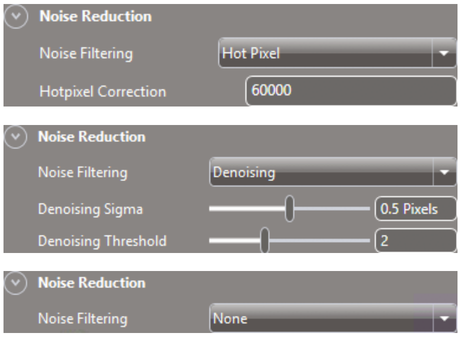
| Control | Function |
|---|---|
|   | **Noise Reduction** for **DCT Data**, choose between the following **Noise Filtering** options:<br>• **Hot Pixel**, set maximum allowed intensity. Higher values are assumed to be outliers and sets to zero,<br>• **Denoising** according to:<br>– **Denoising Sigma**, set 2D Gaussian shape parameter for calculating the smoothed background noise level.<br>– **Denoising Threshold**, set threshold over background noise level, above which intensity is replaced by interpolated value.<br>• **None**, to not apply any noise filtering. |

**Table 3** New Control for the Image Order in Project Tab

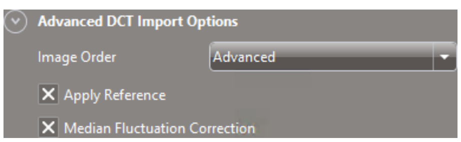
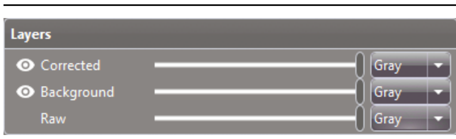
| Control | Function |
|---|---|
|   | **Advanced DCT Import Options** for **DCT Data:**<br>• Change **Image Order** to **Scan Order** if there are sample absorption artifacts in the images that are better reduced by this image order. Usually only applicable for helical phyllotaxis scans. |

**Table 4** Layer Control for the DCT Data Import Preview in Project Tab

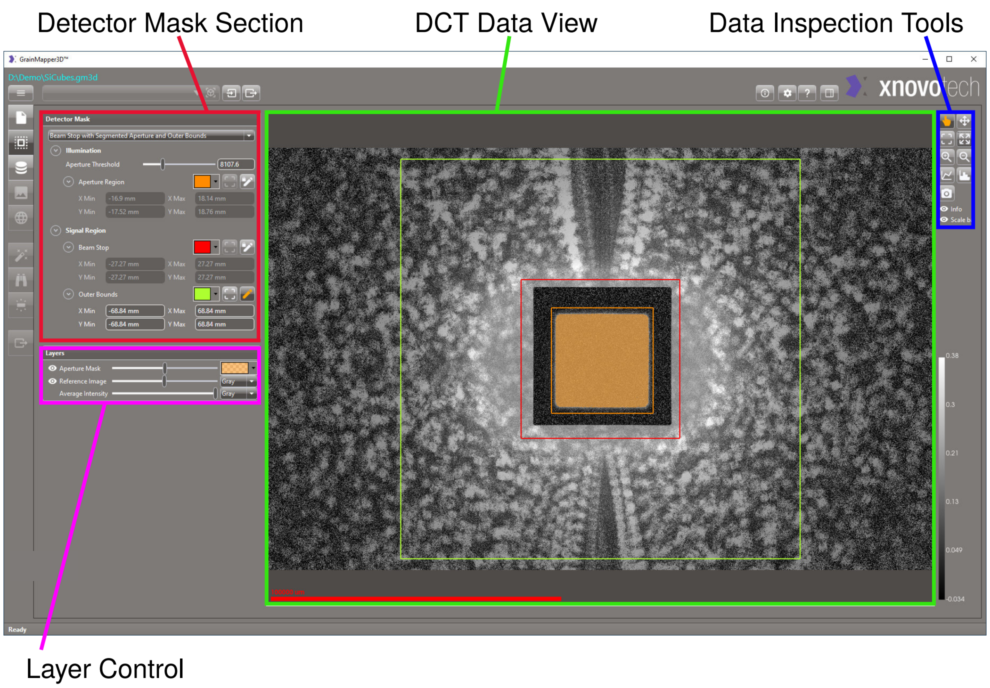
| Control | Function |
|---|---|
|   | **Layers** is the control for visualizing the different corrections applied to the imported **DCT Data**:<br>• **Raw** DCPs (bottom, always shown)<br>• **Background** images for each Raw DCP (middle),<br>• **Corrected** DCPs (top)<br>Use the eye to turn visibility on/off.<br>Use the sliders to change opacity of the layers.<br>Use the drop down boxes to chance colors of the layers. |

## DCT Signal and Illumination Regions

The **Detector Mask** tab is now the second processing step of the GrainMapper3D workflow. The order has been changed in order to exploit the new *aperture illumination* feature when defining the ROI during the absorption data import in the subsequent **Absorption Mask** tab.

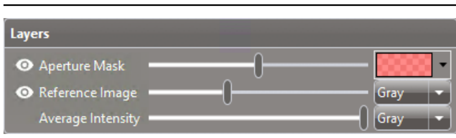
Figure 9 shows the revised layout of the **Detector Mask** tab organized into a data processing **Detector Mask** section, **Layers** control, **DCT Data View** with **Data Inspection Tools**.

**Figure 9** DCT Signal and Illumnation Regions in Detector Mask Tab



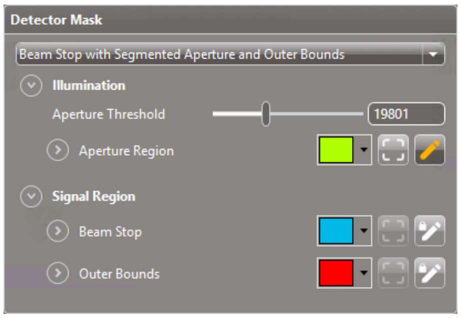
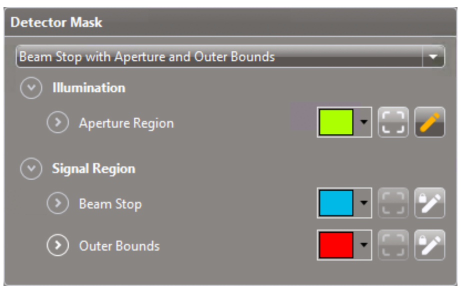
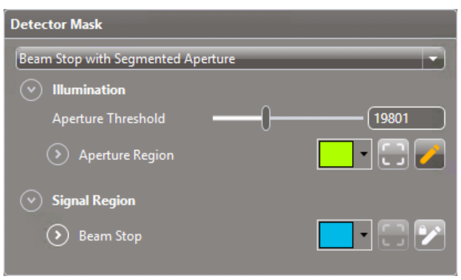
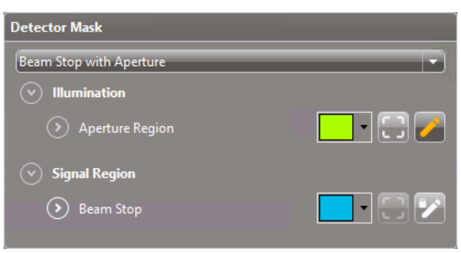
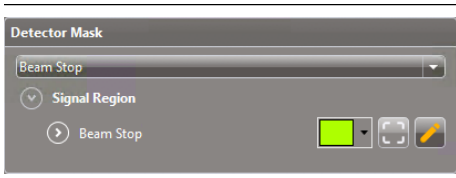

The **DCT Data View** now also shows the **Reference Image** if present. The visual appearance can be adjusted using the **Layers** control as described in Table 5.

**Table 5** Layer Controls of the Detector Mask Tab

| Control | Function |
|---|---|
|  | Use the **Layers** control to visualize:<br>• **Average Intensity** of all DCPs (bottom, always shown)<br>• **Reference Image** (middle)<br>• **Aperture Mask** (top – applies only to **Segmented Aperture**)<br>Use the eye to turn visibility on/off.<br>Use the sliders to change opacity of the layers.<br>Use the drop down boxes to change colors of the layers. |

The first step on the **Detector Mask** tab is to choose the appropriate **Detector Mask Recipe**. The list of detector mask recipes has been revised and the recipes with predefined beam stop sizes have been replaced. The available recipes are listed in Table 6 along with a description of when to use which recipe. Start from the top of the table and choose the first recipe that fits the current DCT Data.

**Table 6** Controls of Detector Mask Tab

| Control | Function |
|---|---|
|  | **Beam Stop with Segmented Aperture and Outer Bounds**, use if:<br>• The aperture illumination is visible through the area covered by the beam stop<br>• The detector signal towards the edges is noisy and/or very weak |
|  | **Beam Stop with Aperture and Outer Bounds**, use if:<br>• The automatic aperture segmentation is not applicable<br>• The detector signal towards the edges is noisy and/or very weak |
|  | **Beam Stop with Segmented Aperture**, use if:<br>• The aperture illumination is visible through the area covered by the beam stop<br>• The detector signal is good all the way to the edges |
|  | **Beam Stop with Aperture**, use if:<br>• The automatic aperture segmentation is not applicable<br>• The detector signal is good all the way to the edges |
|  | **Beam Stop**, use only for:<br>• *Conventional* DCT data where it is not necessary to define the aperture illumination |

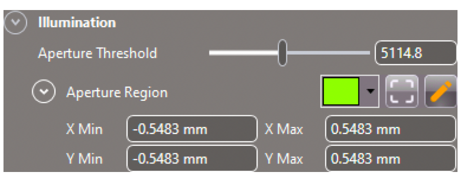
**Illumination – Aperture Region** For any DCT scan where the sample is larger than the aperture FOV, a recipe allowing the user to set the region of direct illumination, defined by the aperture, must be selected. This is done in order to correctly compute which part of the sample is illuminated.

For any *advanced* DCT scan choose a recipe defining the aperture region. It is also recommended to use a recipe with aperture illumination definition for *conventional* DCT scans.

The controls to define the aperture can be seen in Table 7. There are two different recipe types for this:

- **Aperture**, which defines the aperture as a centered box of preset size (375x375um, 250x750um or 750x750um) that can be adjusted by dragging or typing in the boundaries
- **Segmented Aperture**, which allows the user to segment the aperture inside the defined box by setting a threshold.

**Table 7** Controls of the Aperture

| Control | Function |
|---|---|
|  | If the sample ROI is larger than the aperture FOV it is important to define the **Aperture Illumination**, either:<br>• Drag the **Aperture Threshold** slider to set the segmentation threshold for recipes with **Segmented Aperture**<br>• Press [icon] to select one of the predefined apertures<br>• Press [icon] to edit the aperture FOV<br>• Give the boundaries of the aperture |

**Signal Region – Beam Stop** The region on the detector, which is not hit by diffraction spots due to the presence of the beam stop, must be masked out. This must be done for all detector mask recipes.

The beam stop used during acquisition needs to be entered. It is not carried over in the DCT file metadata, as it is mounted manually onto the detector. The predefined beam stops will appear centered, but can be moved and adjusted in size.

The controls to define the beam stop can be seen in Table 8.

**Signal Region – Outer Bounds** Using a detector mask recipe with outer bounds is recommended if the detector signal towards the edges is weak or noisy, for instance due to self-absorption. This usually applies to DCT data collected with a Flat Panel detector.

**Table 8** Controls of the Beam Stop

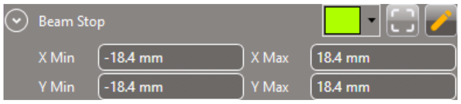
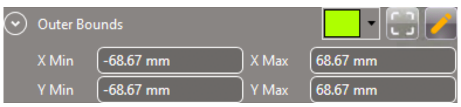
| Control | Function |
|---|---|
|  | Define the **Signal Region** covered by the **Beam Stop**, either:<br>• Press to select one of the preset beam stop sizes:<br>– For the DCT 4X objective<br>– For the Flat Panel detector<br>• Press to edit the beam stop<br>• Give the boundaries of the beam stop |

**Table 9** Controls of the Outer Bounds

| Control | Function |
|---|---|
|  | Define the **Outer Bounds** of the **Signal Region** if the detecor signal towards the edges is noisy and/or very weak, either:<br>• Press for preset values for the Flat Panel detector:<br>– Default Outer Bound<br>– Outer Bounds enclosing 50, 60, 70, 80, 90, or 100% of the detected intensity<br>• Press to edit the outer bounds<br>• Give the boundaries of the outer bounds |

The controls to define the outer bounds can be seen in Table 9. The preset percentile outer bounds are centered on the detector and enclose the named fractions of the detected intensity.

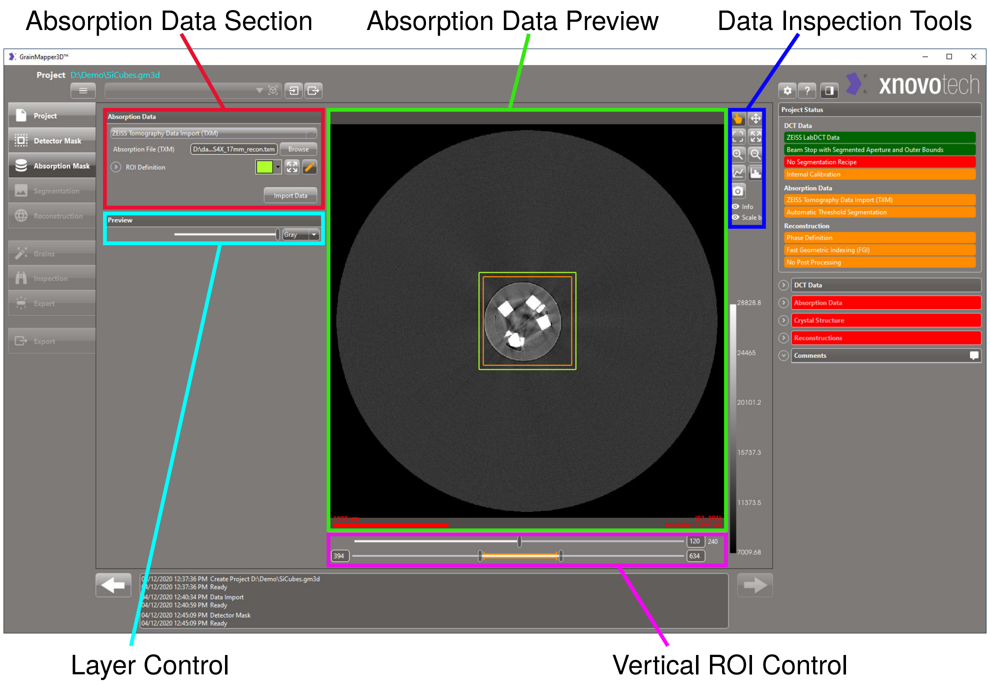
## Absorption Data Import with Preview

The absorption data import, which was previously done in the **Project** tab, has been moved to a dedicated section in the **Absorption Mask** tab. The absorption crop is now done when importing the data. This processing order has the advantage that the *aperture illumination*, defined in the **Detector Mask** tab, now falls prior to the absorption data import, such that the actual illuminated region can be exploited when defining the ROI for the absorption data.

Figure 10 shows the principal layout of the *data import view* of the **Absorption Mask** tab, organized into an **Absorption Data** section for importing data, an **Absorption Data Preview** view with **Data Inspection Tools**, a **Preview** layer control section and a **Vertical ROI Control**.

Table 10 details the control to import absorption data. Once an **Absorption File**

## Figure 10 Absorption Data Import in Absorption Mask Tab

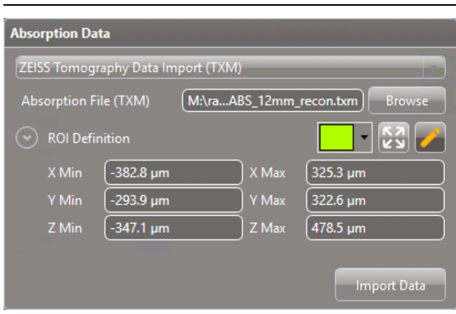



**(TXM)** has been specified, the **Absorption Data Preview** displays the horizontal slice of the absorption data centered in the aperture FOV. The **orange** rectangle on the preview indicates the horizontal aperture FOV, while the ROI Definition is shown in **green**.

The bottom line of the **Vertical ROI Control** corresponds to all vertical slices in the absorption data, the **orange** line segment corresponds to the vertical aperture FOV and the two sliders correspond to the top and bottom ROI limits, which can also be input as slice numbers. The top slider controls the slice preview between the first and last image of the selected ROI.

Figure 11 shows the principal layout of the **Absorption Mask** tab after importing the absorption data.

## Table 10 Controls of Absorption Mask Tab

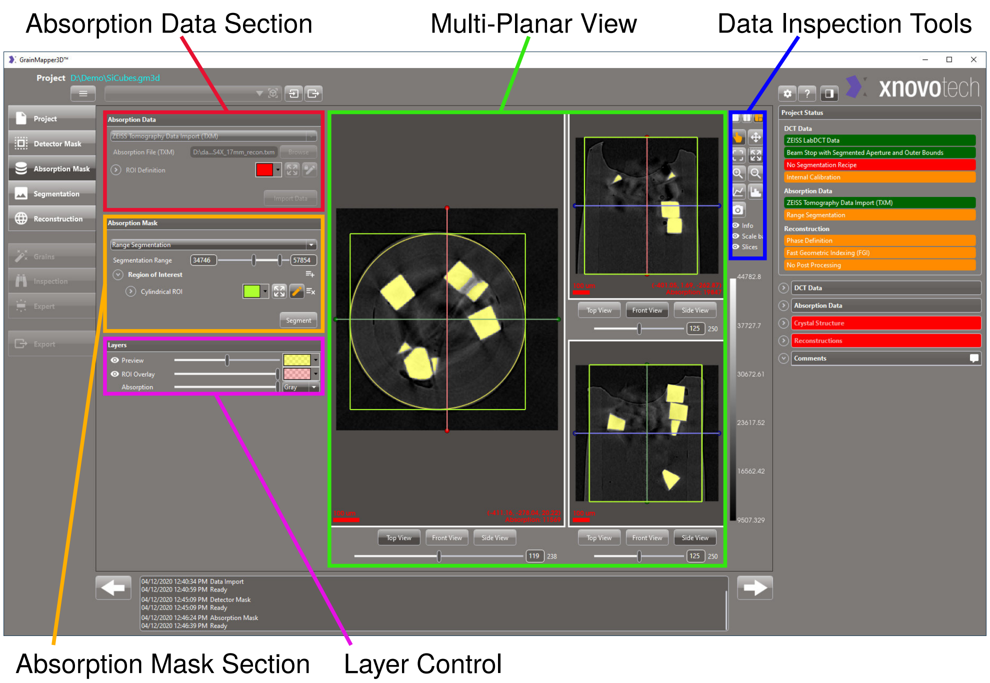
| Control | Function |
|---|---|
|  | ZEISS Tomography Data Import (TXM) imports an absorption volume.<br>To locate the Absorption File (TXM), press Browse.<br>ROI Definition specifies the spatial coordinates of the ROI prior to data import.<br>Press [pencil icon] to freely select the ROI (green) relative to the aperture FOV (orange).<br>Press Import Data to import the cropped *absorption data*. |

# Product Enhancements

## Preview of Absorption Segmentation

The absorption **Threshold Segmentation** and **Range Segmentation** recipe now supports live preview of the chosen threshold or range, respectively. Whenever the threshold or range is changed, a preview layer is updated to indicate which values will be masked. The **Preview** layer can be toggled on or off in the Layer control. However, the live preview only segments individual slices and does not support segmentation filters.

**Figure 11** Absorption Data Segmentation in Absorption Mask Tab




## Other Enhancements

**Importing Combined Segmentation** When importing recipes from another project file, a combined segmentation is now automatically imported together with the depended segmentations without actively selecting them.

**Result File** If the user desires to **Export IPF Color Coding** in the Export tab, it is now possible to choose between two different **Data Types**, namely FLOAT and UINT8. The UINT8 option was added as it corresponds a significant reduction in output file size.

**Visualization** The underlying graphics library has been updated which results in minor rendering improvements.

## User Interface Changes

**Flat Panel Support** Flat Panel data is fully supported in GrainMapper3D 3.0, both as DCT and absorption data. The program automatically detects the detector used and adjusts relevant recipes accordingly, for instance:

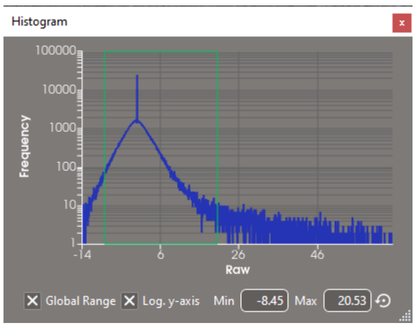
- Preset **Aperture**, **Beam Stop** and **Outer Bound** in the **Detector Mask** tab
- **Self Fitting** parameters and previews in the **Expert** tab

**Project File** The project file format has updated in order to adapt to the new features introduced in GrainMapper3D 3.0. This means that a GrainMapper3D 3.0 project file cannot be opened with any prior version of GrainMapper3D. Vice versa, if the user attempts to open a prior GrainMapper3D 2.x project file in GrainMapper3D 3.0 a warning will be issued that the file format is about to change. It is recommended to open prior GrainMapper3D project files as read-only in GrainMapper3D 3.0 to preserve the prior file format or to make a copy_v3.gm3d before opening.

**Project Status** The recipes listed in the **Project Status** section have been rearranged into the groups **DCT Data**, **Absorption Data** and **Reconstruction** to accommodate the new processing workflow.

**Histogram control** The histogram controls when importing DCT or absorption data now have a **Global Range** checkbox as shown in Figure 12. Check to preserve the data range when changing processing parameters or slicing through the data sets.

**Figure 12** Histogram Control with Global Range




**New Preferences** A few additional preferences have been added, allowing the user to tailor the new recipes in the user interface, namely:

- Preferred **Background Correction** and **Noise Reduction** recipes for **DCT Data Import**.
- Preferred **Data Type** for **Export IPF Color Coding**.

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**GrainMapper3D™**
Release Notes

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