

Release Notes

GrainMapper3D™ 2.3

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



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New Features

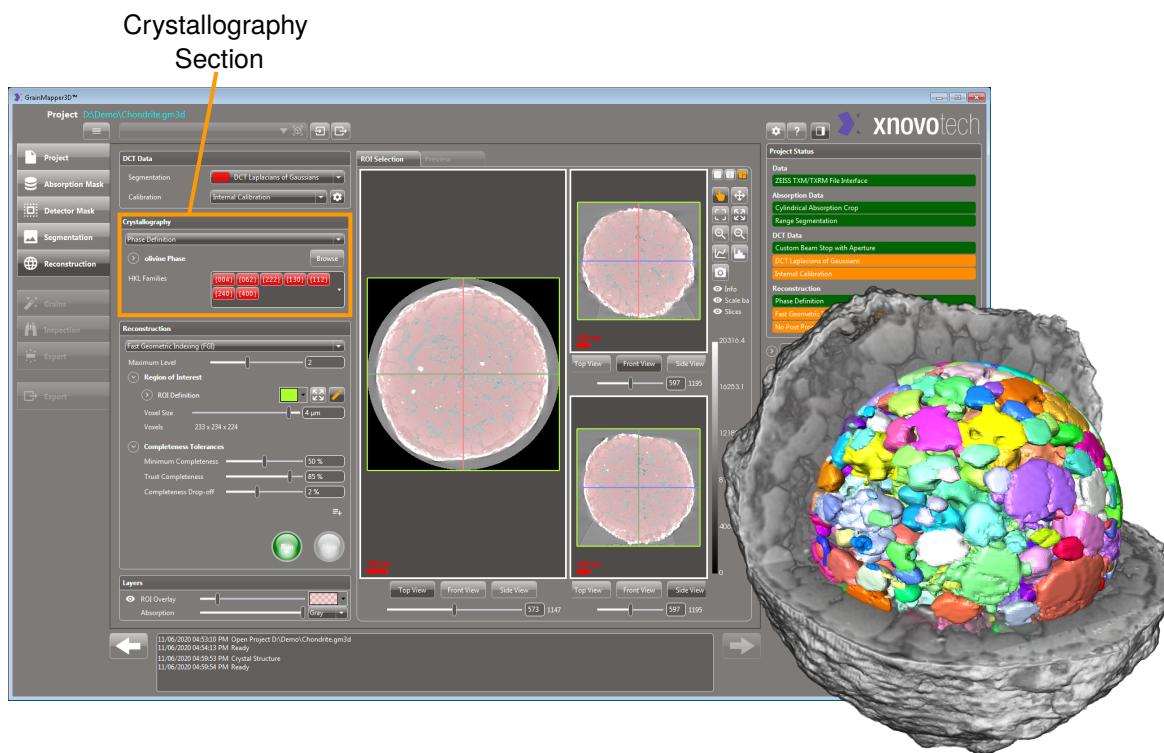
All Crystal Symmetries

This release of the GrainMapper3D enables orientation indexing with any crystal system from triclinic to cubic.

Each reconstruction now carries over its own crystallographic information, such that the phase can be changed from reconstruction to reconstruction¹. This allows quicker testing of different lattice parameters for non-cubic materials, where the axis ratio of the unit cell impacts indexing.

The **Crystallography** section has been moved from the **Project** tab to the **Reconstruction** tab as shown in [Figure 1](#). Additionally, The **CIF (Crystallographic Information File)** recipe has been replaced with a new **Phase Definition** recipe detailed in [Table 1](#).

Figure 1 The New **Reconstruction** Tab



The new recipe allows to customize the selection of families of lattice planes used for indexing. The **HKL Families**, as shown in [Figure 2](#), can be sorted by **Multiplicity** $M[\#]$, **Structure Factor** $|F|^2$ or **d-spacing** $d[\text{\AA}]$ by pressing on the column headers. However, an appropriate choice of **HKL Families** is required in order to

¹This was previously only allowed if all reconstructions had been removed, since the crystal structure was treated globally

Table 1 New Controls of The **Reconstruction** Tab

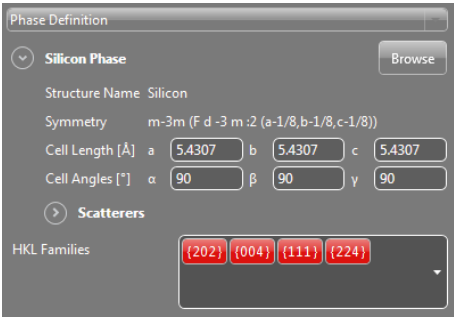
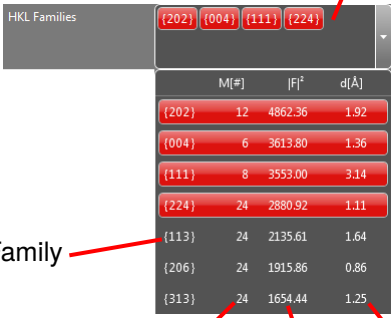
Control	Function
	<p>Phase Definition imports a CIF-File. Press Browse to locate a file. When importing a crystal structure a default choice of HKL Families is made, which will be used for indexing.</p> <p>In order to change the selection of HKL Families press the drop down of the menu and select appropriate lattice plane families from the list. Press one of the column headers multiplicity $M[\#]$, structure factor $F ^2$ or d-spacing $d[\text{Å}]$ in order to change sorting.</p> <p>See also Figure 2 for the drop-down.</p>

Table 2 Recommended Number of Lattice Planes by Crystal System and Bravais Lattice Type

Crystal system	Laue class	P	A, B, C	I	F
triclinic	$\bar{1}$	>15			
monoclinic	2/m	>10-11	>9-11		
orthorhombic	mmm	>9	>7-9	6-8	6/8
trigonal	$\bar{3}, \bar{3}m$	5-7			
tetragonal	4/m, 4/mmm	6-7		4-6	
hexagonal / rhombohedral	6/m, 6/mmm	4-6			
cubic	$m\bar{3}, m\bar{3}m$	4		3	4

Figure 2 Selection of **HKL Families**

Selected Families



Family	Multiplicity	Structure Factor	d-spacing
{202}	12	4862.36	1.92
{004}	6	3613.80	1.36
{111}	8	3553.00	3.14
{224}	24	2880.92	1.11
{113}	24	2135.61	1.64
{206}	24	1915.86	0.86
{313}	24	1654.44	1.25

achieve reliable orientation indexing with lower crystal symmetries. [Table 2](#) lists the recommended number of lattice planes by crystal system and Bravais lattice types Primitive (P), Base-centered (A, B or C), Body-centered (I) and Face-centered (F). As a rule of thumb, the multiplicity of all selected families should sum up to be >30 to guarantee a unique orientation indexing solution up to the ambiguity given by the Laue class. By default, an automatic choice of **HKL Families** is made according to the highest structure factors. Consequently, the **Number of HKL** parameter of the **Fast Geometric Indexing (FGI)** has been removed.

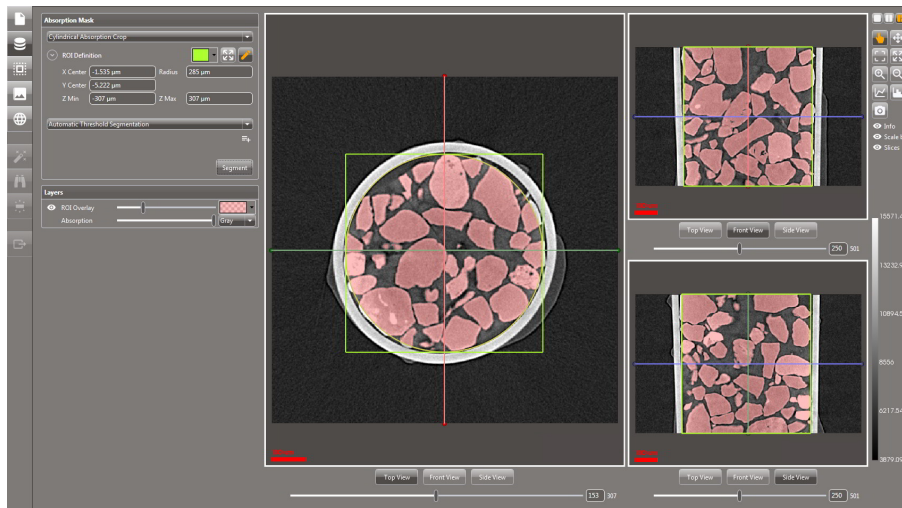
Projects created with GrainMapper3D v2.2 or earlier will be automatically upgraded to the new **Phase Definition** recipe when opening the project file.

Advanced Absorption Segmentation

Tools to improve the absorption segmentation have been added. All absorption segmentation recipes now uniformly use filters that can be added on demand. Changes are described below and usage is detailed in [Table 3](#).

Cylindrical Absorption Crop The **Cylindrical Absorption Crop** recipe allows to crop out an upright cylinder in the absorption volume. This can be useful when dealing with cylindrical samples or samples encased in a capillary or Kapton tube as demonstrated in [Figure 3](#).

Figure 3 Example Screen of a Cylindrical Absorption Crop



Absorption Range Segmentation A new absorption segmentation recipe **Range Segmentation** has been added, which allows to segment absorption data with a lower and an upper threshold. This can be useful for samples showing absorption contrast like displayed in [Figure 4](#).

Marker Based Components A marker allows to extract individual connected components of the segmented absorption mask. For instance, this can be used to remove noise from the segmentation as demonstrated in [Figure 4](#).

Figure 4 Absorption Range Segmentation with Marker Based Component

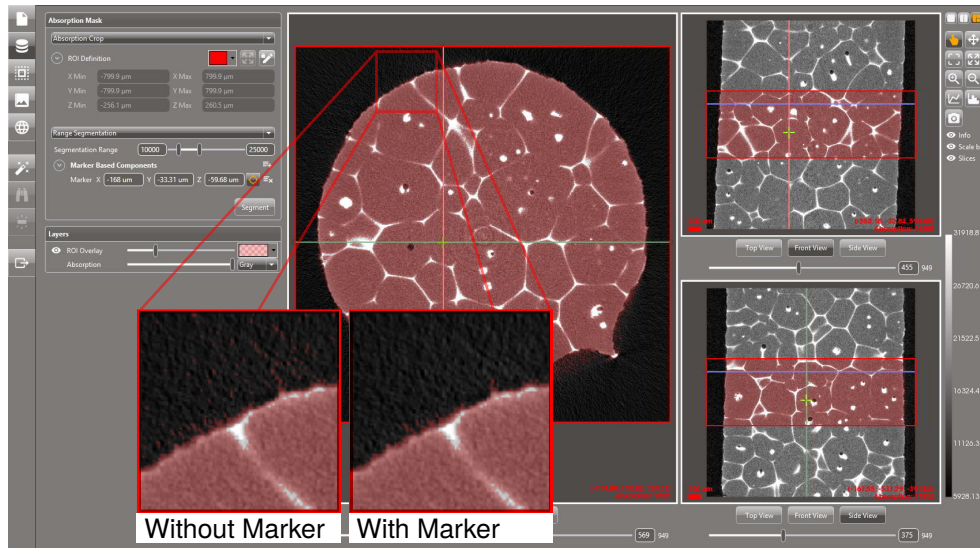
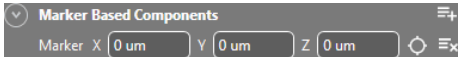



Table 3 New Controls of The **Absorption Mask** Tab

Control	Function
	<p>Cylindrical Absorption Crop crops the imported absorption volume by a cylindrical region of interest and fills values outside of the cylinder with zeros.</p> <p>ROI Definition specifies the cylinder given by center, radius and spatial position of the cylinder bases.</p>
	<p>Range Segmentation performs a threshold segmentation of the absorption volume based on a user specified lower and upper threshold.</p>
	<p>Press Add Filter and select a filter from the drop-down list in order to add a processing filter.</p> <ul style="list-style-type: none"> • Fill enclosed regions, check to omit unwanted holes within the segmented volume. The function will use a seed growing algorithm in order to obtain a full volume.

Table 4 New Controls of The **Absorption Mask** Tab (continued)

Control	Function
	<ul style="list-style-type: none">• Marker based components, select Marker and<ul style="list-style-type: none">– Enter the coordinates of the marker directly, the coordinates can be read out of the Multi-Planar View (MVP) by moving the mouse over the component of interest.– Press the Locate button next to the coordinate input in order to locate the marker in the MVP. The MVP will automatically go to the slices in which the marker is located and enabled it for dragging. Click and drag the marker in the MVP to the region that should be extracted. <p>Press Remove Filter  next to the filter in order to remove the processing filter.</p>

GrainMapper3D Viewer

The **GrainMapper3D Viewer** application can show *Result* or *Project Files* containing *Reconstructions* created with GrainMapper3D. The viewer shown in [Figure 5](#) is organized in a **Viewer Toolbar**, **Data Section**, **Multi-Planar View**, **Data Inspection Tools** and a **Layer Control**. The controls behave like known from the **Grain** tab of the GrainMapper3D. The **Data Section** provides information about the **File Version**, the **Absorption Volume** and the **LabDCT Volume** contained in the *result file*.

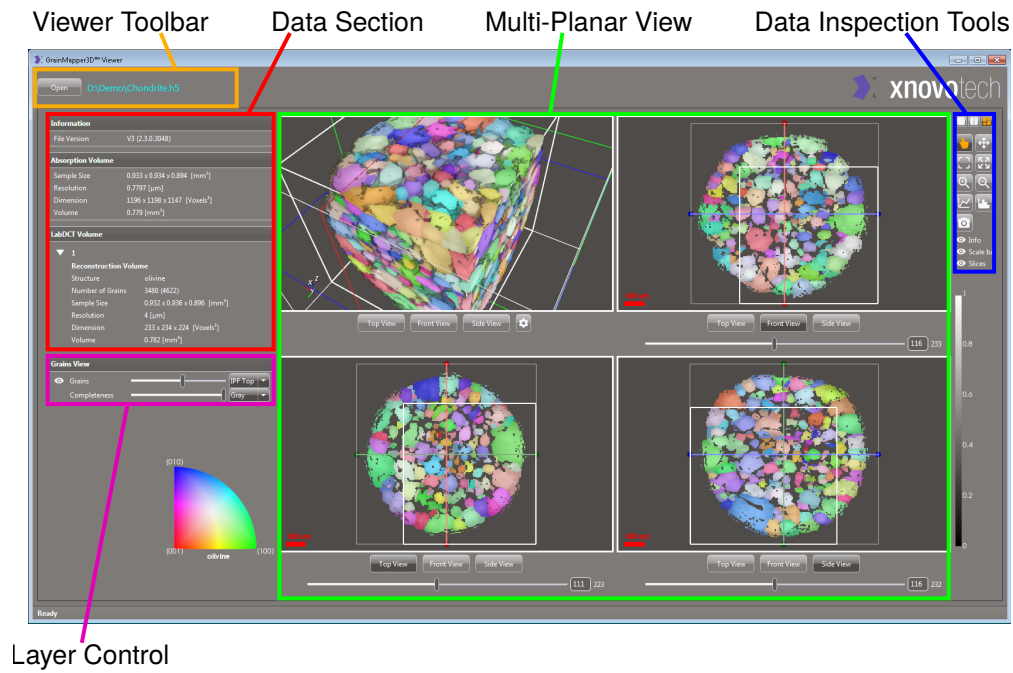
In order to show a *Reconstruction* with the viewer application select **Start > All Programs > Xnovo Technology ApS > GrainMapper3D Viewer** from the **Windows Start** menu. The **GrainMapper3D Viewer** window opens. Press the **Open** button. A Windows **Open File** dialogue appears. Choose a result or project file and press **Open**. The viewer will load and display the specified file.

Product Enhancements

Absorption Data Import

The **ZEISS TXM/TXRM File Interface** now supports the import of cropped and rotated absorption volumes created with the Scout-and-Scan Control System Reconstructor version 15 or higher. Data collected with a prior version must be reconstructed with version 15 in order to get the correct spatial location of a cropped volume and make use of this feature.

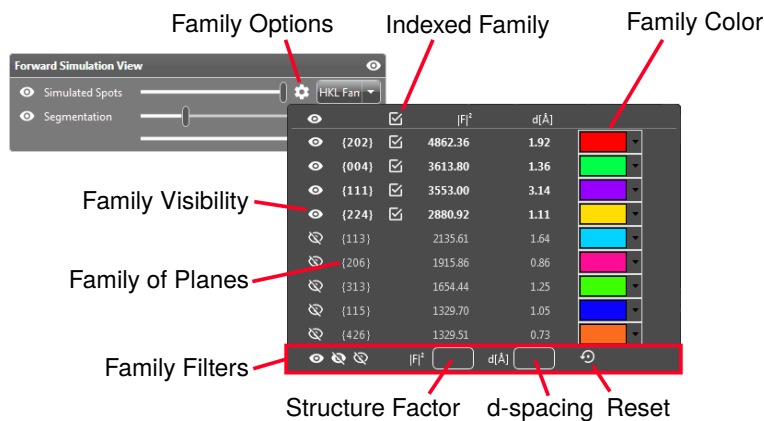
Figure 5 GrainMapper3D Viewer showing a *Result File*



Forward Simulation

The *forward simulation* of the **Inspection** tab is now computed on the fly for each projection. This removes the overhead after performing a grain definition and also allows to reopen *Projects* containing a reconstruction more quickly. Additionally, the **Family Options** menu shown in Figure 6 has been revised and now shows besides the **Structure Factor** also the **d-spacing** of each family and indicates whether the family was used for indexing or not. The families can be sorted by structure factor or d-spacing by pressing the column header accordingly. **Family Filters** allow to quickly show all, show only indexed or hide all families. Entering a **Structure Factor** or **d-spacing** will expand or reduce the list to the minimum value given.

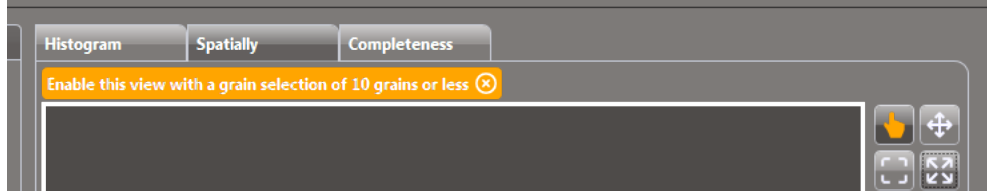
Figure 6 Forward Simulation of Lattice Plane Families



Other Enhancements

Grain Selection The performance when switching between several grain selections with a lot of grains was significantly improved. In turn, on the **Expert** tab plotting the residuals spatially will be only enabled when 10 or less grains are selected like mentioned in [Figure 7](#).

Figure 7 Grain Selection Warning on **Expert** Tab

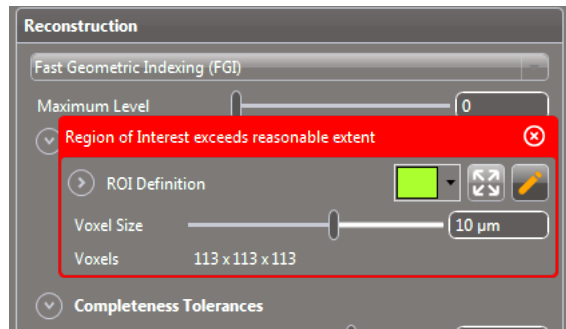


Visualization The underlying graphics library has been updated. All 2D / 3D views have been refurbished getting faster and better rendering with smoother interaction.

User Interface Changes

Error Messages They can be removed by pressing the close button in the upper right corner as shown in [Figure 8](#).

Figure 8 Removable Error Message



Histogram Computation The histogram computation better accounts for outliers in the data which enhances contrast of displayed value range.

Screenshots Taking a screenshot on the **Grain** tab now also saves the IPF colormap.

Absorption Tab Dragging of the ROI in the MVP does not snap to voxel boundaries any more but shows the coordinates defined. Voxel centers which fall inside the ROI are considered to be part of the ROI.

Reconstruction Tab When resizing the ROI of the absorption crop on the **Absorption Mask** tab and going to the **Reconstruction** tab the ROI for indexing will be resized automatically if it does not have reasonable extent anymore.

GrainMapper3D™

Release Notes

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