GrainMapper3D™ 2.2

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

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Contents

New Features

Advanced Segmentation

The advanced segmentation provides improved segmentation capabilities covering a larger variety of diffraction contrast patterns.

It is now possible to filter spots based on several feature properties and also to combine several segmentations. This allows better extraction of diffraction peaks and their shapes. For instance for a bimodal grain size distribution as artistically illustrated in Figure 1, leading to grain maps with higher completeness and sharper grain boundaries.

Figure 1 Artistic Illustration of Advanced Segmentation
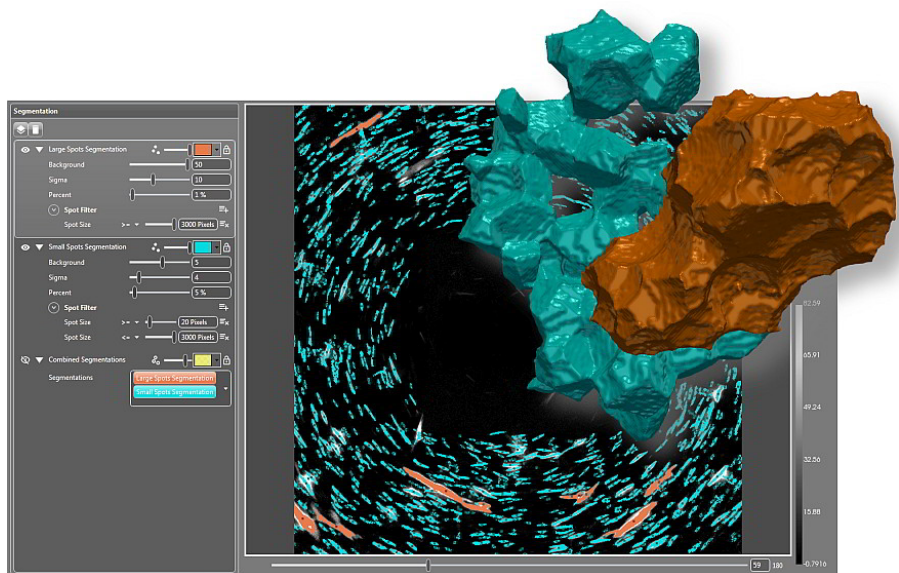
Spot filters The ability to filter segmented spots based on their size, shape or intensity.

In order to add a spot filter press **Add Spot Filter** and choose an appropriate entry from the drop-down list as shown in Figure 2a. An overview of all available spot filters is given in Table 1. The comparison operator for each filter can be selected, reading

"Property [greater / greater equal / equal / smaller equal / smaller] Value"

as also shown in Figure 2b. A spot filter can be removed by pressing **Remove Spot Filter** next to the filter.

Spot filters have been added to all segmentation recipes (except combined segmentation), replacing their previous equivalent filter as listed in Table 2.
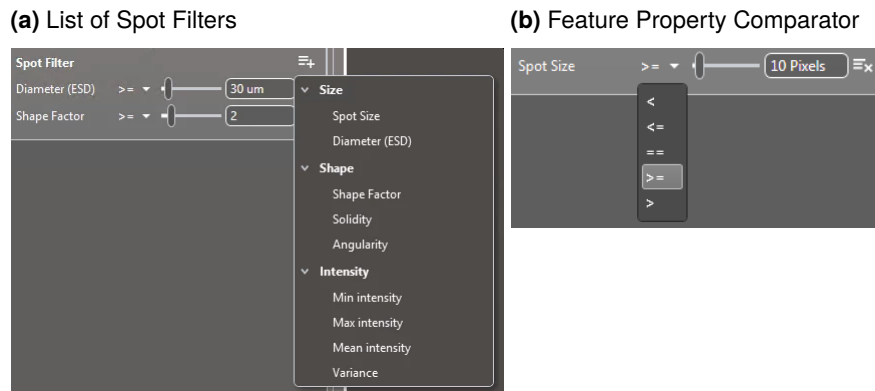
Figure 2 Spot Filter

(a) List of Spot Filters   **(b)** Feature Property Comparator

Table 1 Description of Spot Filters

| Spot Filter	Description
Spot Size	Measures the number of pixels of a spot
Diameter (ESD)	Equivalent spherical diameter of a spot in microns
Shape factor	Ratio of the Eigenvalues of major and minor principal axes a and b of a spot
Solidity	Ratio of spot area divided by its convex hull area
Angularity	Angle α between direction of principal major axis and image centre
Min, Max, Mean intensity	Intensity value of a spot
Variance	Variance of all intensity values of a spot
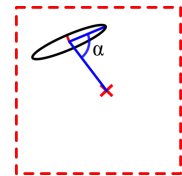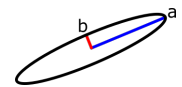
Table 2 Renaming of Filters (Default Value in Brackets)

Segmentation Recipe	Old Name	New Name
DCT Line Filter	Area (25 pixels)	Spot Size (>=25 pixels)
	Shape (0)	Solidity (>=0.1)
DCT Laplacian of Gaussians	Minimum spot size (10)	Spot Size (>=25)

Spot Centroids   Sometimes it is difficult to distinguish whether two spots have been properly separated or one spot is split into several (Figure 3b). Press the **Spot Centroid Button** (3a) in order to investigate whether a spot is properly segmented and only one centroid has been assigned (Figure 3c).

Figure 3   Centroid Overlay in the DCT Data View

(a) Spot Centroids Button

(b) Not separated

(c) Separated
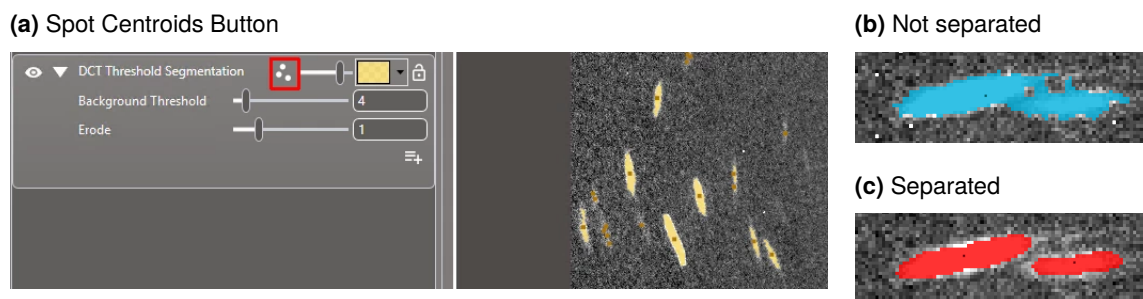
New Segmentation Recipes   The following segmentations have been added:

- **DCT Threshold Segmentation**, an intensity erosion and threshold is applied to the diffraction images.
- **Combine Segmentations**, several segmentations can be combined with a logical or operation to one binary image

For details of the controls, please see Table 3.

Preferences

User preferences allow to customize GrainMapper3D settings in order to simplify the workflow for frequently recurring tasks:

- Project, set an author name that will be used when creating a project or adding comments.
- Performance, set performance settings for the GrainMapper3D.
- Appearance, set customized colours and font sizes for segmentations or plots.
- Screenshot, set preferred image export format and compression options
- Paths, set where CIF-files or DCT Data will be located by default.
- Recipes, set default options for some recipes.

In order to open the Preferences press the **Preferences Button** ⚙ in the upper right corner as shown in Figure 4.

A detailed information of the corresponding controls is given in Table 4.
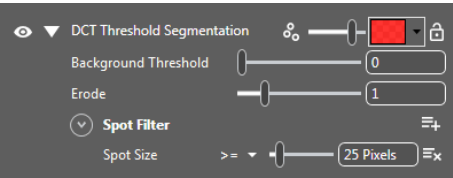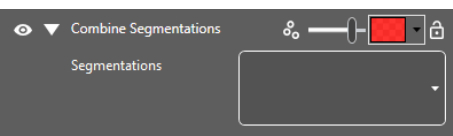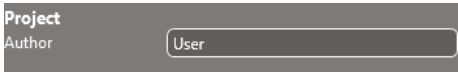
Table 3 Controls of New Segmentation Recipes
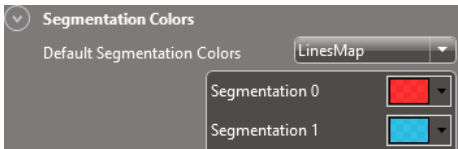
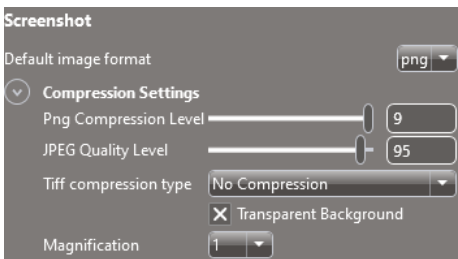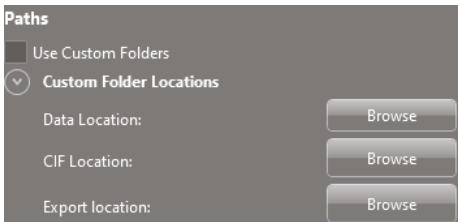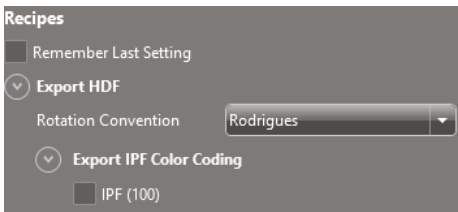| Control	Function
	DCT Threshold Segmentation performs a morphological erosion with given size on the DCT projection and thresholds the filtered image to remove artefacts. • **Background Threshold** is the intensity value to threshold after applying the erosion kernel. • **Erode** is the kernel size $2n + 1$ to use for the image erosion. Default filters: • The **Spot Size** is the minimum number of pixels that a spot needs to have.
	Combine Segmentations, allows to combine arbitrary segmentations from the list of segmentations. Selected segmentations will be combined by a *binary or* operation. The spot centroids of all segmentations will be combined, but no centroids of the resulting spots will be computed. • In order to add a segmentation press the drop-down of the **Segmentations** parameter and select one or multiple segmentations in the list. • Unselect a segmentation from the drop-down in order to remove the segmentation.

Figure 4 Preferences

Table 4 Controls of Preferences

Control	Function
Project / Author: User	Enter an author name that will be used when creating a project or adding a comment to a project.
Performance / Number of Cores: 8 / Remember Number of Cores	**Number or Cores** (logical CPUs) on workstation to be utilized for reconstructing a grain map. Use **Remember Number of Cores** option, in order to remember setting on the next start-up.
Segmentation Colors / Default Segmentation Colors: LinesMap / Segmentation 0 / Segmentation 1	Choose or edit **Default Segmentation Colors** that will be assigned when creating a new segmentation on the **Segmentation Tab**.
Plot Settings / Font Size: 12 / Annotation Color / Plot Color / Plot Foreground Color	Set the **Font Size** on all 2D and 3D Plots. Select a **Annotation Color** to change the colour of the scale bar and info text in the plot. Choose a **Plot Color** to change the colour of the plot, e.g. Histogram. Choose a **Plot Foreground Color** to change the colour e.g. for the Line Profile.
Screenshot / Default image format: png / Compression Settings / Png Compression Level: 9 / JPEG Quality Level: 95 / Tiff compression type: No Compression / Transparent Background / Magnification: 1	Choose a **Default image format** from the drop-down list to be **png**, **jpg**, **bmp** or **tiff** when creating a screenshot. Adjust compression settings if required. Screenshots will have the size of the current display. Choose a **Magnification** in order to enlarge the screenshot by given factor.
Paths / Use Custom Folders / Custom Folder Locations / Data Location: Browse / CIF Location: Browse / Export location: Browse	**Use Custom Folders** will open the file dialogue at given location, if specified, otherwise will attempt to open at last known location, for: • **Data Location**, pointing to the folder where data is usually located • **CIF Location**, pointing to the folder containing all CIF files • **Export Location**, pointing to the folder where PDF reports or result files should be stored.
Recipes / Remember Last Setting / Export HDF / Rotation Convention: Rodrigues / Export IPF Color Coding / IPF (100)	Check **Remember Last Setting** if the last setting used in the user interface should be remembered for the recipes given below. Otherwise, the option of the recipe parameters listed below will be used as default value.

Product Enhancements

CIF (Crystallographic Information File)

A CIF now states a detailed error if it can not be imported, e.g. if the scatterer is unknown.

Segmentation Cache

A cache for the segmentation preview was added. When browsing through DCT images in the DCT Data View or adjusting parameters, already temporarily computed segmentations will be immediately displayed flicker-free.

Segmentation Persistence (Cache)

All segmentations used to index DCT data are now persisted to disk in a hidden folder ".gm3d/projectfilename" next to the project file. This allows faster reopening of project files and also faster switching between reconstructions employing different segmentations. If the folder was deleted it will be restored automatically (if possible). Moving project files to different places will thus affect performance when recomputing the segmentations is required.

When opening project files created with older versions of GrainMapper3D (in write mode), they will be updated accordingly to support the segmentation persistence.

Indexing

The implementation of the *Fast Geometric Indexing* reconstruction algorithm has been further optimized and gained a speed-up, in certain situations up to 50%. The memory handling was improved, now allowing reconstructions with a finer discretization down to 1um or 1024³ voxels, though a discretization <256³ voxels is still the recommended choice.

Indexer Options

The option to add an additional shift to the absorption reconstruction data relative to the DCT data was added. Some acquisition system show a systematic offset between those two reconstructions, though a careful calibration was performed.
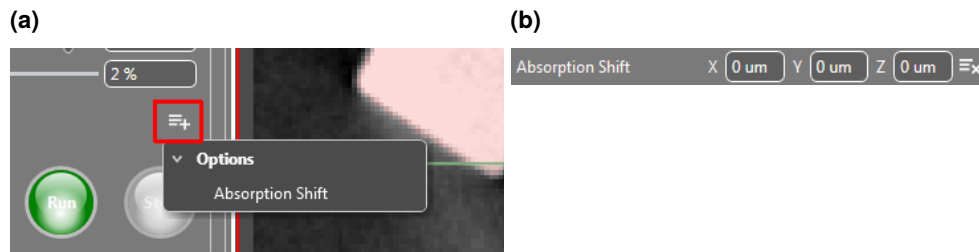
In order to add an additional shift to the absorption data press **Add Options** ⊞ and select **Absorption Shift** from the drop-down list as shown in Figure 5. Enter a shift that the absorption mask will be translated in the reconstruction volume relative to the DCT reconstruction.
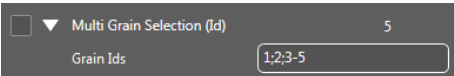
Figure 5 Indexer Options

Export Data

Optionally select IPF direction (100), (010) or (001) for orientation colour coding to be exported.

Grain Selection

Added a new grain selection by *Grain Id* called **Multi Grain Selection (Id)**, which allows to select individual grains. The *Grain Id* can be read out in the planar sections of the multi-planar view of the inspection tab. For details, please see Table 5.

Table 5 Controls Added to the Inspection Tab

Control	Function
	Multi Grain Selection (Id) selects all grains with: • **Grain Ids** listed in the text field. Use ';' in order to enter multiple grain ids. Use '-' to select a range of grain ids.

User Interface Changes

Drag-and-Drop support

Added support to drag files from the *Windows Explorer* directly into GrainMapper3D as shown in Figure 6a. Dragging a single or a pair of TXM/TXRM files into the project manager will create a new project. CIFs, TXM or TXRM files can be directly dragged into the recipe accordingly.

Added support to rearrange segmentation layers in the DCT Data View by drag-and-drop segmentations in the Segmentation Tab as shown in Figure 6b. The rearranged segmentation order will not be persisted to the project file and is only temporary.

Figure 6   Drag-and-Drop Support

(a) Windows Explorer   **(b)** Segmentation Tab
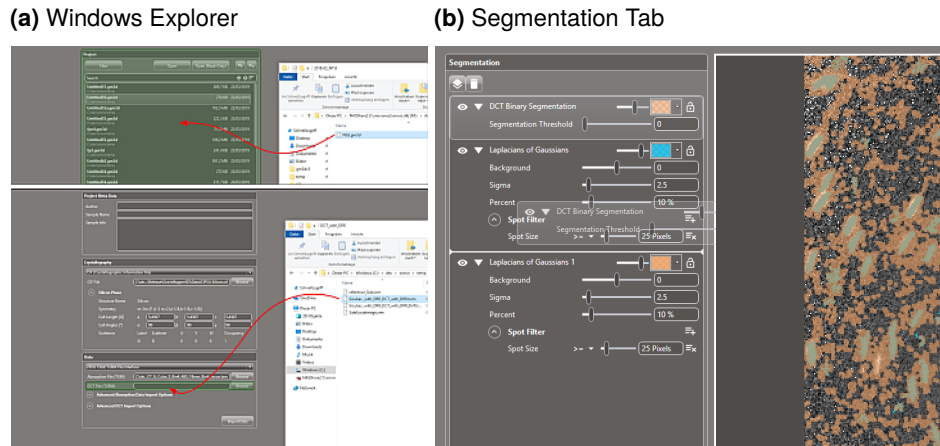

Other Changes

Replaced Icons for the Reconstruction Manager, Recipe Import and Export of the **Project Toolbar** icons.

Removed the About Tab and added a **Settings Toolbar**, which gives access to Preferences, Help & Support. The Maximize Main Window button hides the Project Status and Engine Info when toggled to give a data centric view.
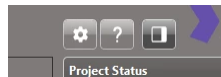
Added segmentations colours to the DCT Data selection on the Reconstruction Tab as shown in Figure 7, in order to have an easier overview of which segmentation will be actually used.

Figure 7   Segmentation Colours
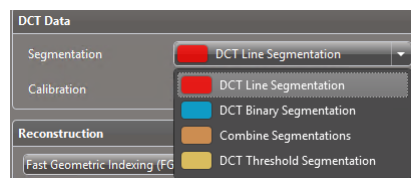
GrainMapper3D™
Release Notes

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