

IndexLaue: program to analyze Laue diffraction data

Copyright (C) 2022 Evgenii Vasilev (UNH), Dmitry Popov (HPCAT)

Evgenii.vasilev@unh.edu

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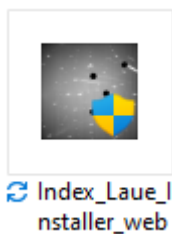
Limitations

The software should be run on a display with effective resolution of at least 1920x1080 pix. Note that display scaling (125%, 150%, etc.) changes the effective resolution. For example, if a display has a native resolution of 1920x1080 pix, 150% scaling will result in the effective resolution of 1280x720 which will be too less for IndexLaue to display properly. In this case, scaling should be adjusted to achieve the effective resolution of at least 1920x1080 pix.

If the software window does not fit into the screen, increase the display resolution or decrease scaling. In Windows 10/11, this can be done in Options-Display-Scale/Display resolution.

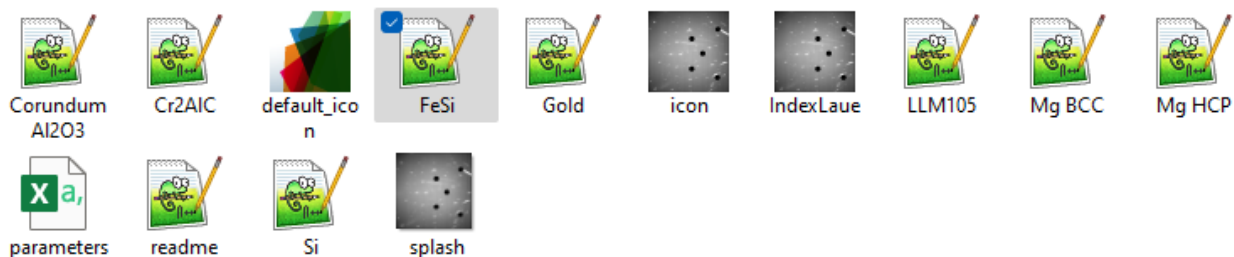
Installation

Launch the web-installer of Index Laue



and follow the installer's guidance. During first installation, MATLAB libraries will be downloaded that can take ~10-15 minutes.

When the installation is finished, the app can be located in the folder (default): **C:\Program Files\IndexLaue\application** . The folder contains an executable file "IndexLaue.exe" and material files with .txt extension such as "Mg HCP.txt", "Gold", "FeSi". These material files are later used for input of the crystal structure for indexing.



Scan parameters tab

Once the software is launched, enter scan parameters

The screenshot shows the 'Scan parameters' tab of a software interface. At the top, there are four tabs: 'Scan parameters', 'Image processing', 'Mapping', and 'Indexing'. Below the tabs, there is a button labeled 'Select folder with scans'. Underneath this button is a section titled 'List of folders:' which contains a list of folders with checkboxes: 2021-2, 2021-3, FeSi, HPCAT, Mg_Vasiliev, Optical_images, Scan1 (checked), Scan2, Scan3, and Scan4. Below the list, there are input fields for 'Number of background frames' (set to 10), 'Square scan' (checked), and 'Scan dimension' (set to 21 by 21). Further down, there is a section titled 'Setup geometry' with a button 'Select a file with Dioptas geometry'. Below this button is a text field for 'Calibration file' containing the path 'C:\Users\aveil\OneDrive - USNH\Documents\high pressure\data\2021-3\Calibration\CeO2_29p2keV_x7_y0_2t30_144.poni'. Below the text field are input fields for 'Shift of omega axis from mono beam, mm' (0.01), 'Detector pixel size, mm' (0.2), 'Detector image size, pix' (2048), and 'Beam energy, keV' (5 to 90).

Select folder with scans: Select a "root" folder that contains folders with scans. For example, this can be folder "C:\Laue Data\" that contains folders with scans "scan1", "scan2", etc.

In the **"List of folders"** select folder(s) of interest. **Limitation:** if multiple folders are selected, they should have equal number of images (.tif files) and equal number of background frames.

Number of background frames: Number of background frames recorded on the detector (typically 10).

Square scan: check the box if the scan has equal number of rows and columns, for example, 15x15. If there is only 1 image selected, it is also considered "square" with 1 row and 1 column.

Scan dimension: if scan is not square, manually enter number of columns (left field) and number of rows (right field).

Setup geometry:

Select a file with Dioptas geometry: click to select a calibration file extracted from Dioptas. This file has an extension .poni and differs from experiment to experiment.

Calibration file: displays the selected Dioptas file.

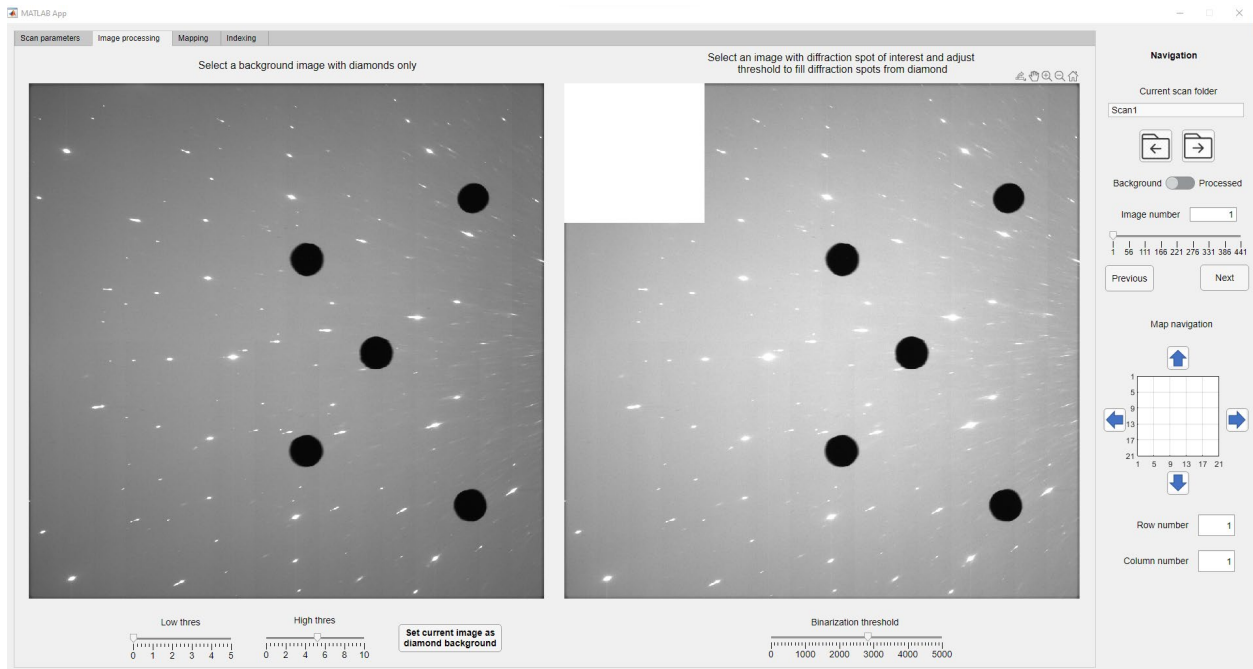
Shift of omega axis from mono beam, mm: do not change unless specified (default value 0.01).

Detector pixel size, mm: do not change unless specified (default value 0.2).

Detector image size, pix: do not change unless specified (default value 2048).

Beam energy, keV: do not change unless specified (default value 5 to 90 keV).

Image processing tab



Using “**Low thres**” and “**High thres**”, adjust brightness and contrast of the image. **Limitation:** value of “**High thres**” should always be higher than “**Low thres**”.



Using navigation panel, select a background image with diffraction spots from diamonds only. This image will be used to subtract diamond background. See an example of a good background image below.

Navigation panel

Navigation


Current scan folder

Scan1

Background ☐ Processed





Image number



1 56 111 166 221 276 331 386 441

Previous Next

Map navigation

1 5 9 13 17 21

1 5 9 13 17 21

Row number

Column number

Name of the current folder

If multiple folders are selected, click these buttons to swap between those folders.

Switch between navigation control of background and processed image

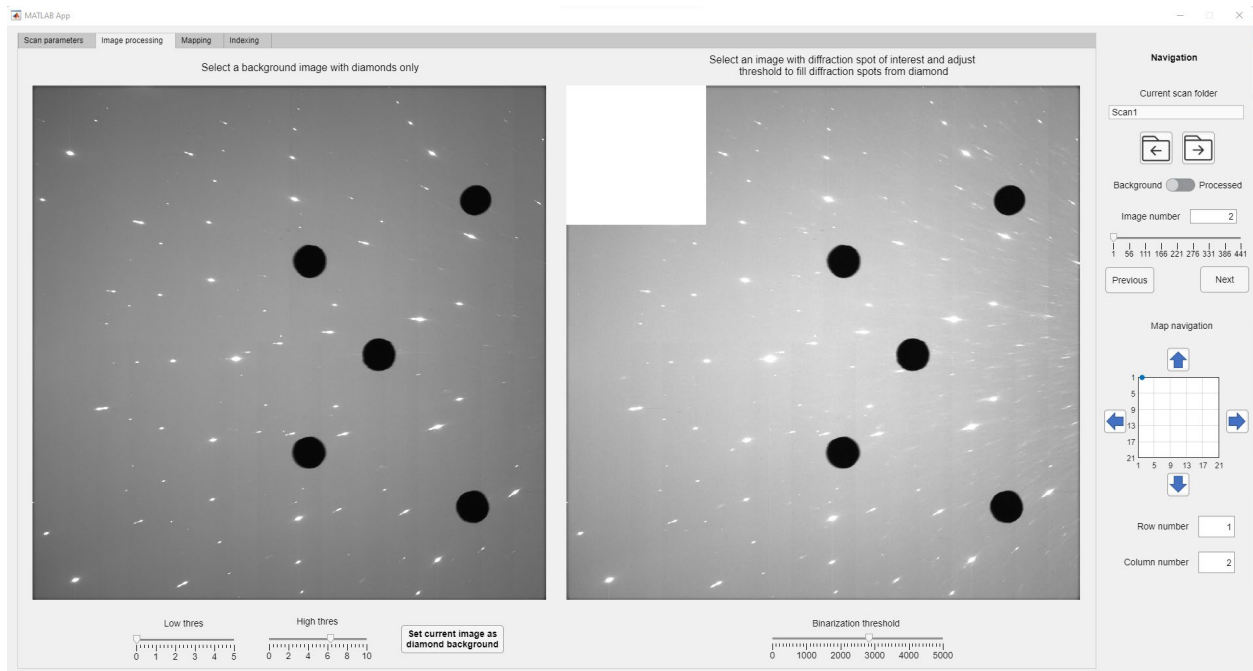
Choose image number by manually typing in the field, moving the slider, or clicking **“Previous”/“Next”**

Alternatively, navigate images by moving around the map

Or selecting a row and column number

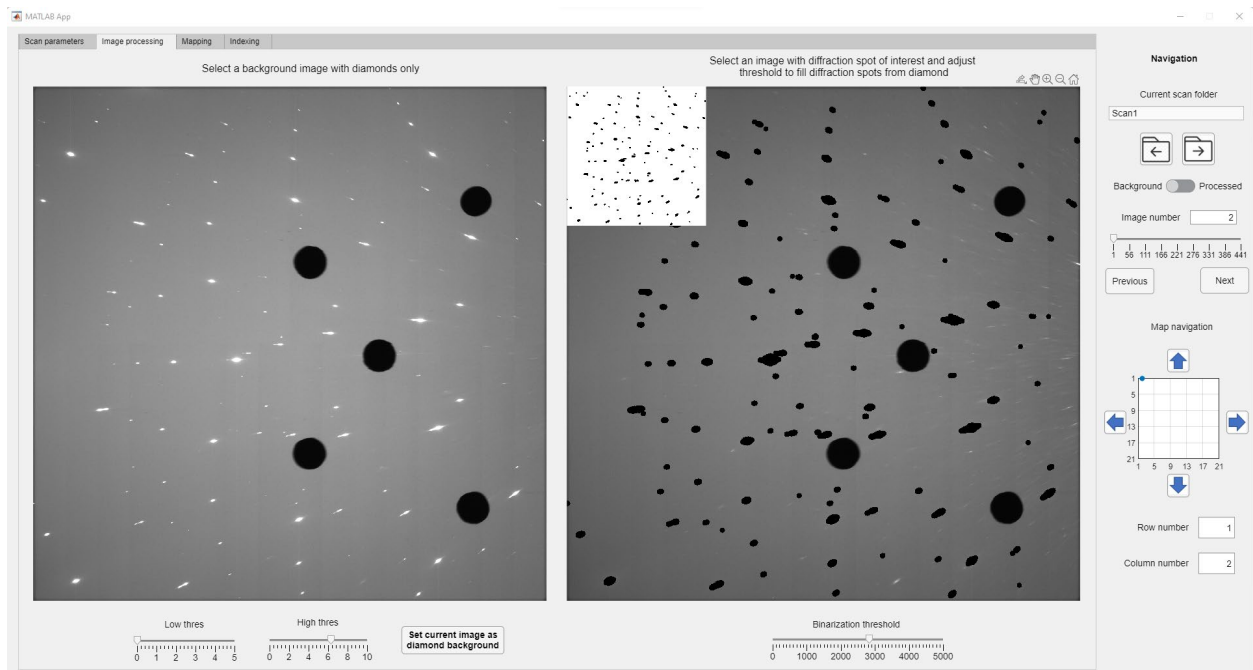
Image processing (continued)

Once the image with reflections from diamonds is located, for example:



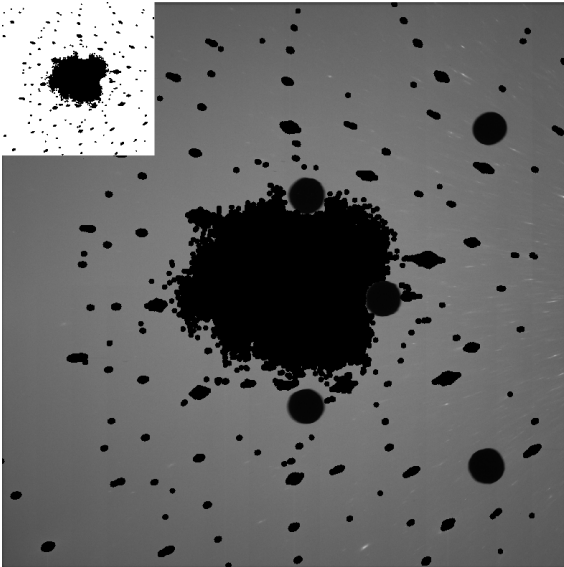
click **“Set current image as diamond background”**

The diamond background will be subtracted from the right “processed” image:

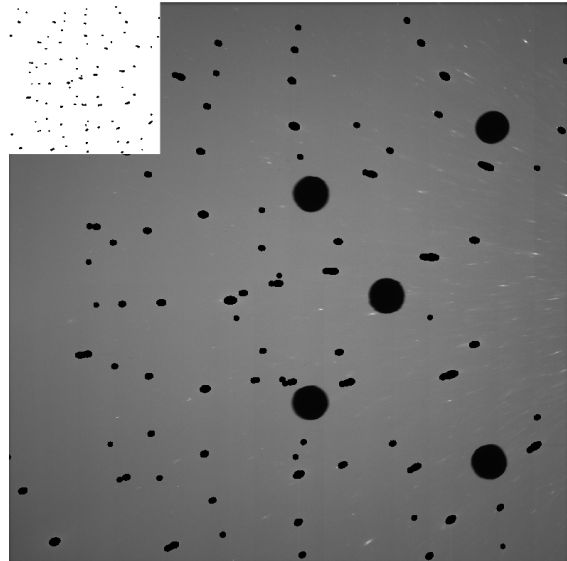


Black and white image in the top-left corner of the processed image shows the selected mask.

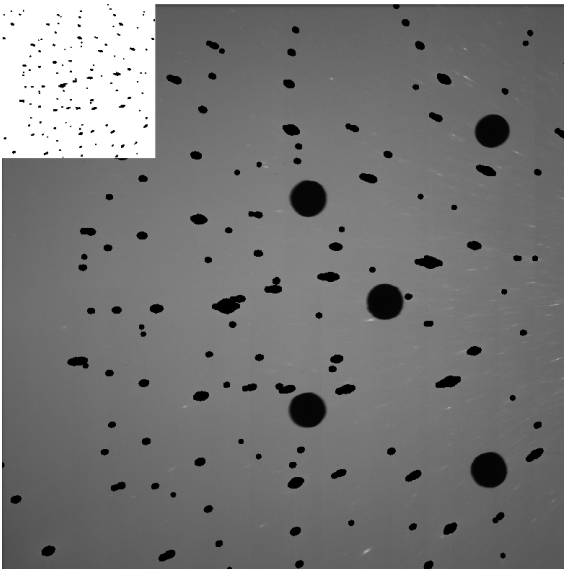
Adjust binarization threshold in a way that it fills as many diamond reflections as possible without oversaturating the background.



Binarization threshold is too low – area in the middle is flood-filled.



Binarization threshold is OK but could be reduced a little bit to fill more diamonds



Optimal binarization – almost all diamond reflections are masked.

After binarization is adjusted, switch navigation control to the processed image by clicking the switch

Background ☐ Processed

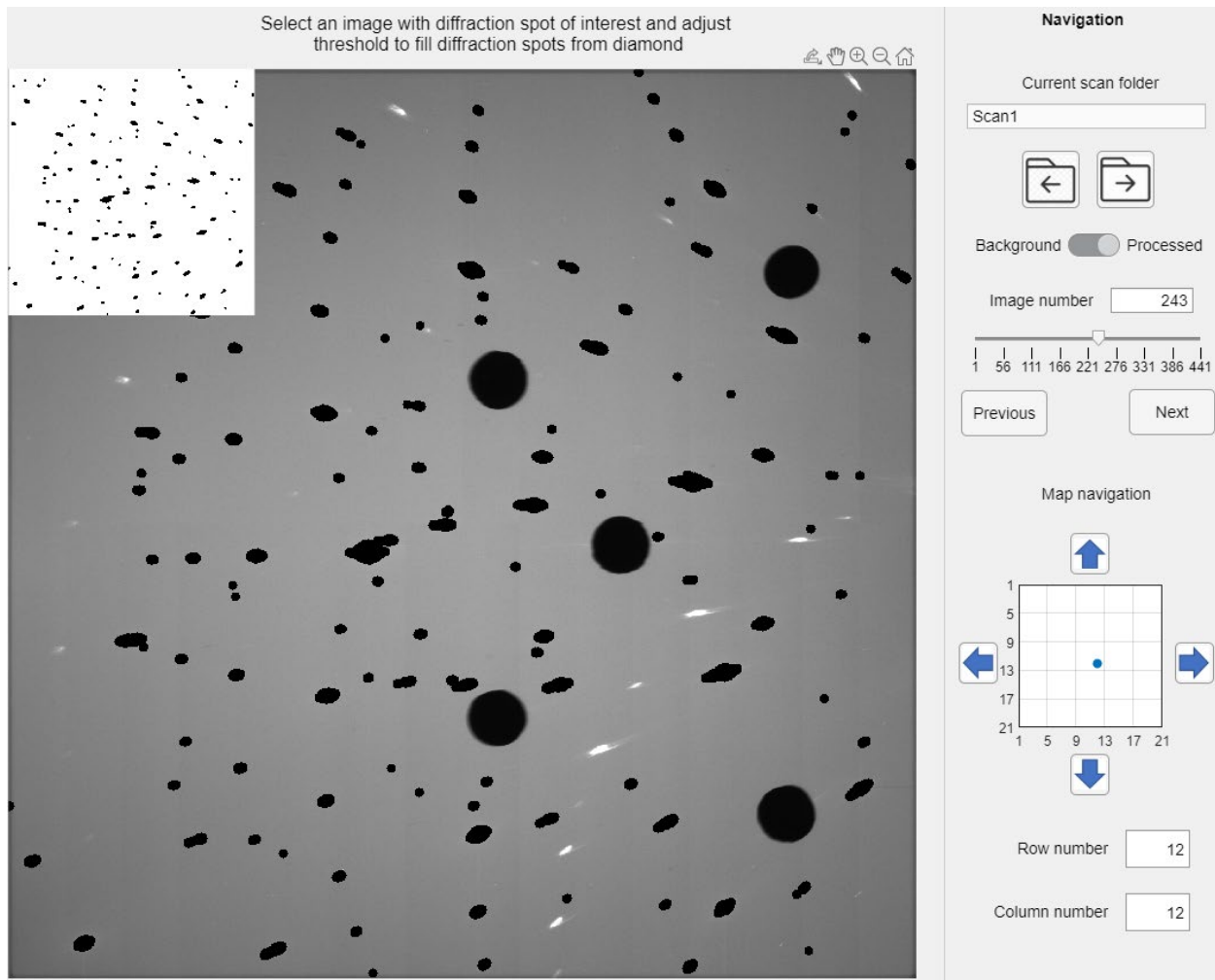
or left-mouse-clicking on the right image.

The image number is reset to 1 and now navigation panel will control the processed image number.

Left mouse click on the background image will change navigation control to background image.

Find an image with diffraction spots of interest:

Select an image with diffraction spot of interest and adjust threshold to fill diffraction spots from diamond



Navigation

Current scan folder
Scan1

Background ☐ Processed

Image number

1 56 111 166 221 276 331 386 441

Previous Next

Map navigation

1 5 9 13 17 21

1 5 9 13 17 21

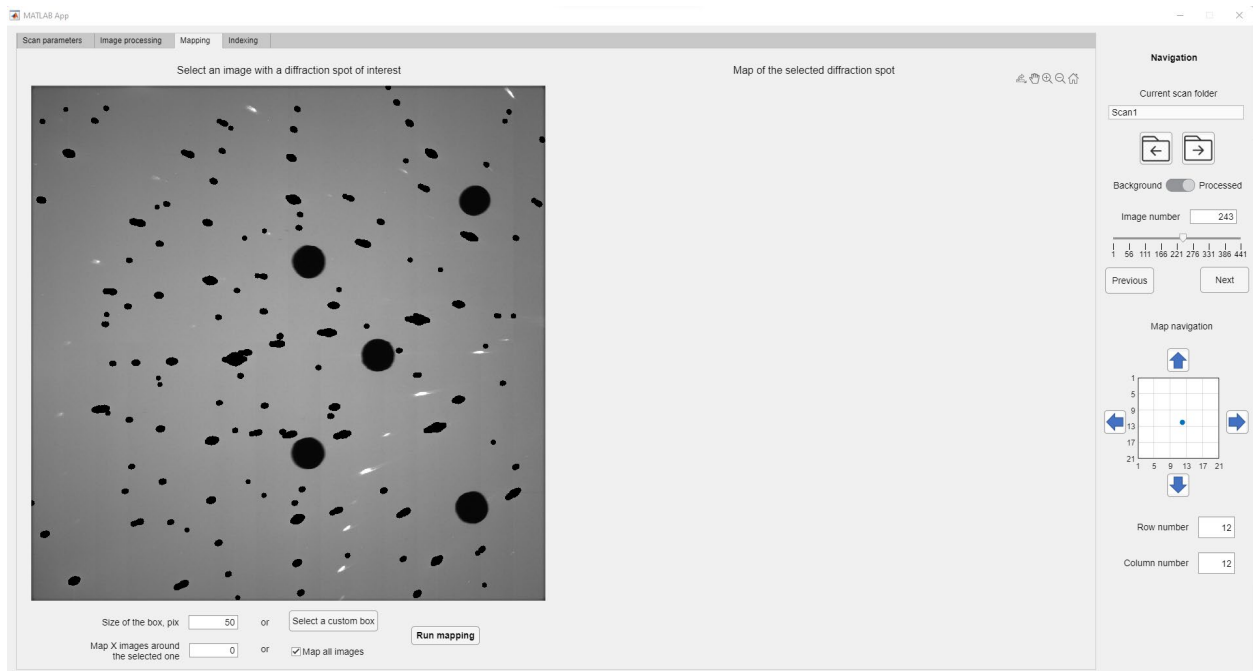
Row number

Column number

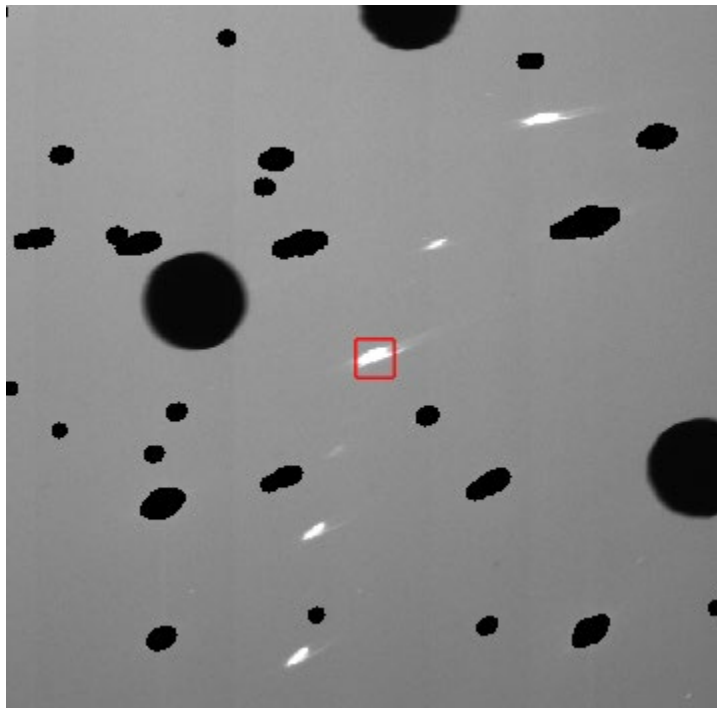
This image will then be used for mapping and indexing.

Mapping

Go to the “Mapping” tab:



Left mouse click on the detector image to select an area for mapping

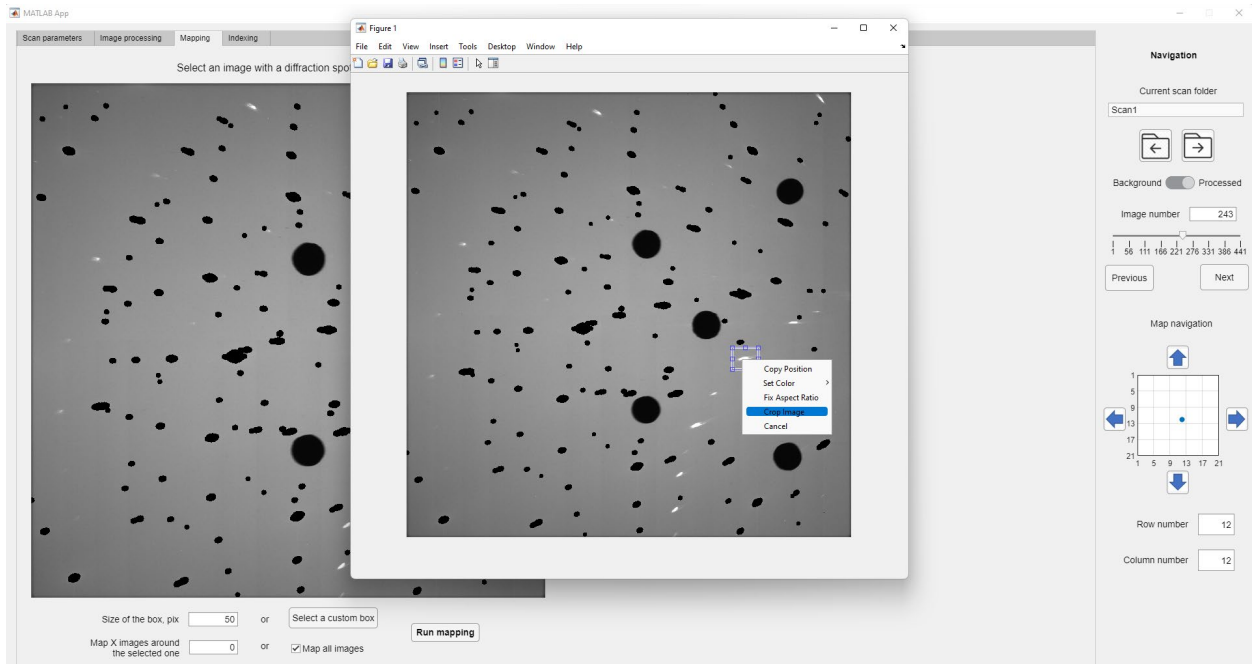


Adjust size of the selection box: Size of the box, pix

To select a rectangular and non-square area, click

Select a custom box

Select a custom area, right mouse click on the image and select “Crop image”



One area is selected, choose either to map all images and enter an integer number in the field

☒ Map all images

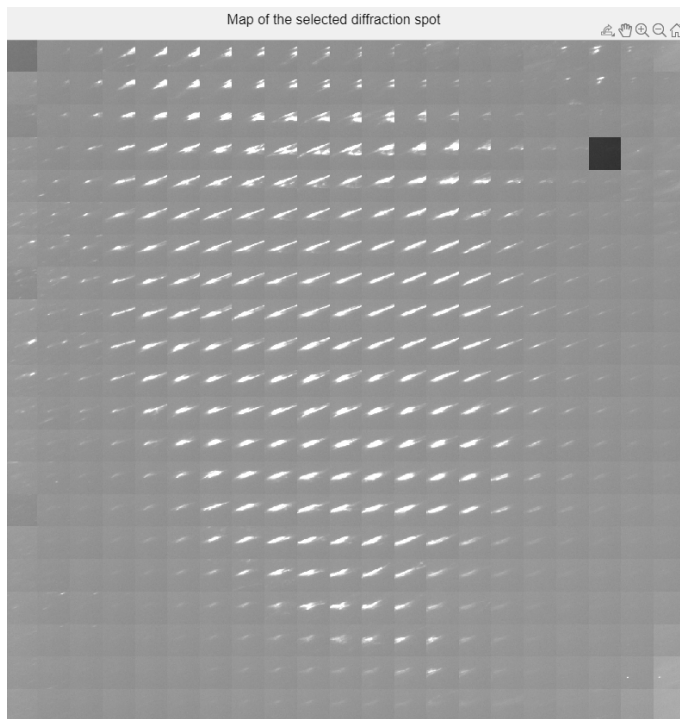
or unclick this checkbox

Map X images around the selected one

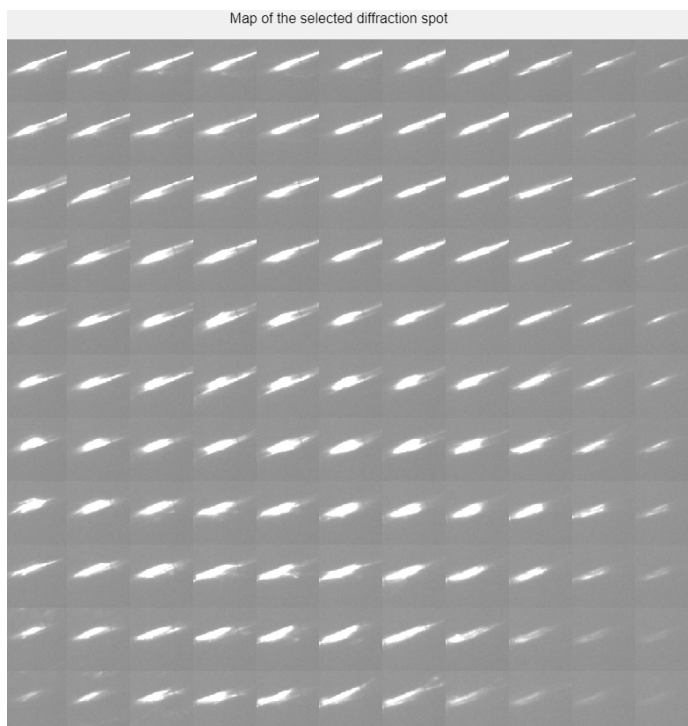
to map X images around the selected one.

Click “Run mapping”

“Map all images” will create a 2D map of the entire dataset:

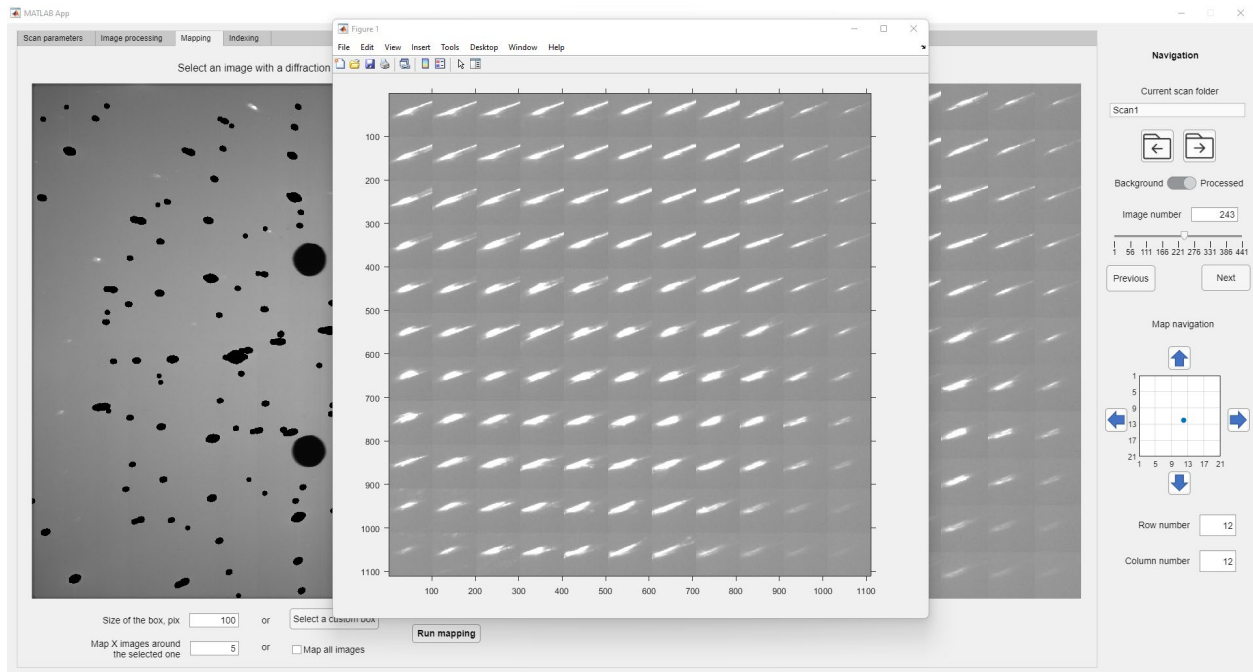


“Map X image around the selected one” will create a local map around the current image. For example, below is a map of 5 images around the selected one (row 12, column 12). A total map of 11 x 11 images is created.



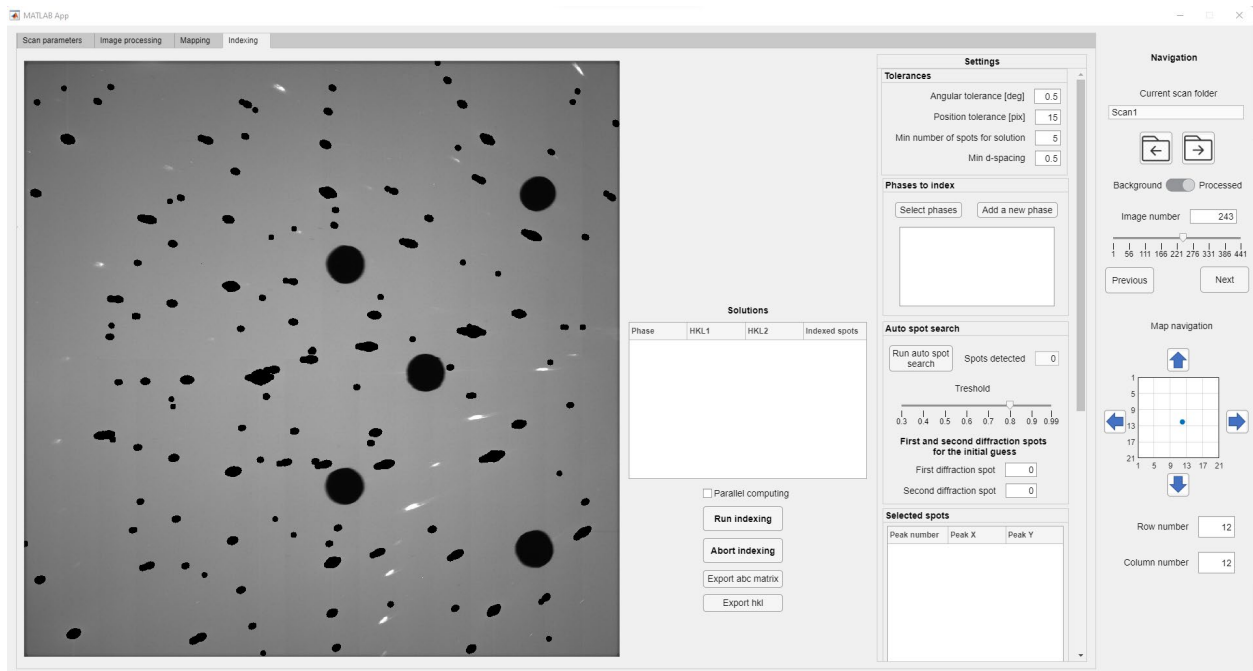
The map is saved into the folder with the current scan data. If the next time this scan folder is loaded, the created map will be automatically loaded and displayed.

Left mouse click on the map to open it in a separate window with a scale bar, drag and zoom functionality:



Indexing

Go to the “Indexing” tab:



Define tolerances:

Tolerances	
Angular tolerance [deg]	<input type="text" value="0.5"/>
Position tolerance [pix]	<input type="text" value="15"/>
Min number of spots for solution	<input type="text" value="5"/>
Min d-spacing	<input type="text" value="0.5"/>

The typical values are:

Angular tolerance: 0.1-0.5 deg.

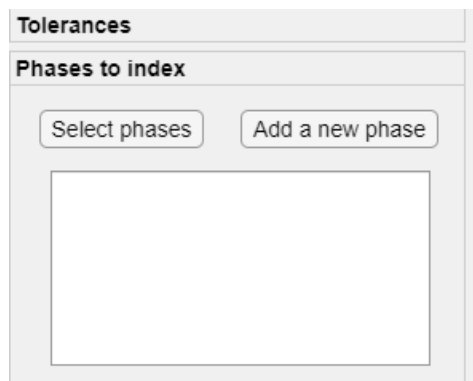
Position tolerance: 5-15 pix.

Min number spots for solution: 5 (normally not changed unless specified).

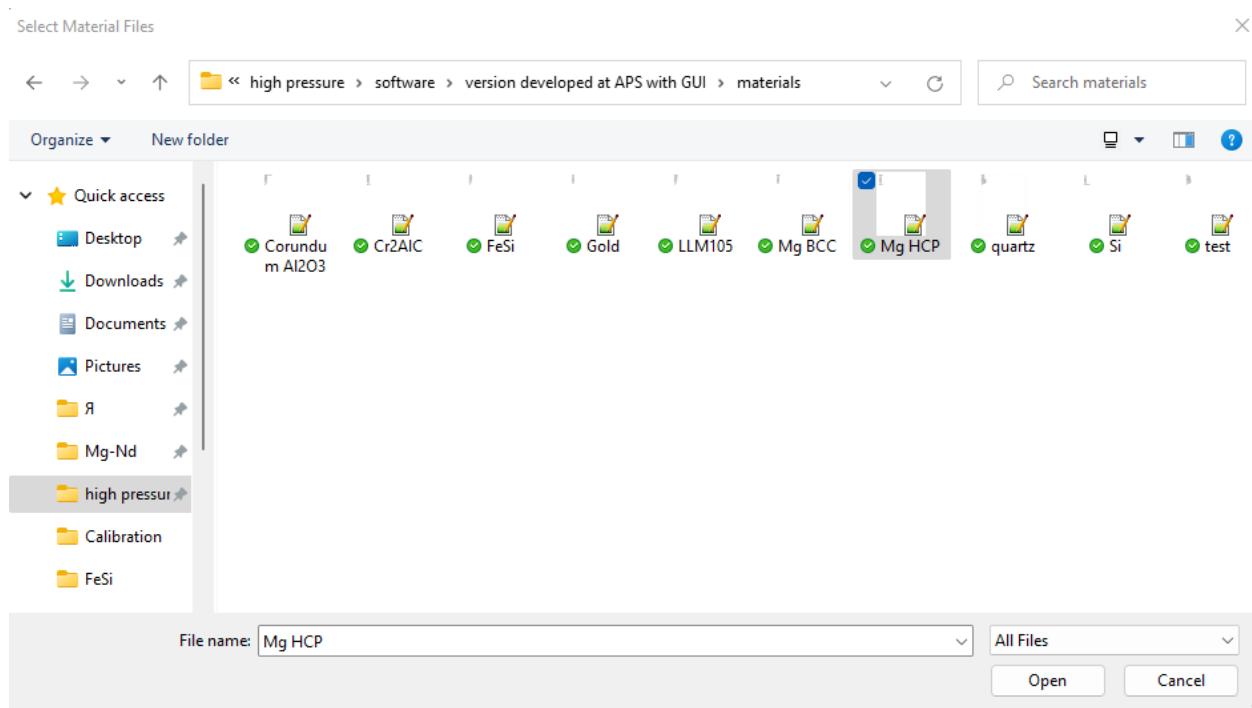
Min d-spacing: depends on the material, larger for larger lattices.

Relaxed tolerances will provide more solutions at a cost of increased computation time.

Click on the title “Tolerances” (or any other title of a tab) to minimize/maximize the tab:

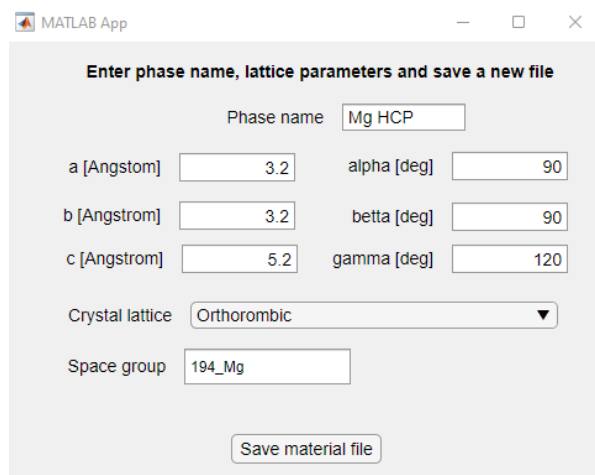


Next, click “Select phases”



Select one or many materials files.

If you do not have one for your material, instead click “Add a new phase”. A new window pops up:

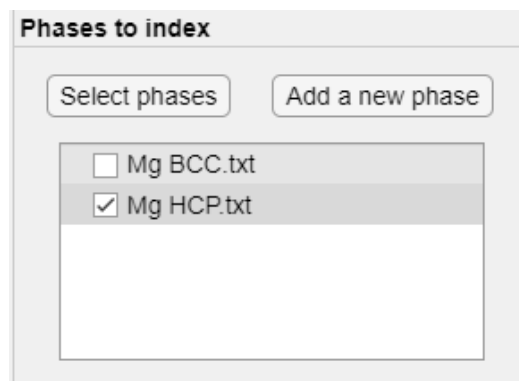


The image shows a MATLAB App window with the title bar 'MATLAB App'. The main content area has a title 'Enter phase name, lattice parameters and save a new file'. It contains several input fields: 'Phase name' with the text 'Mg HCP', 'a [Angstrom]' with '3.2', 'alpha [deg]' with '90', 'b [Angstrom]' with '3.2', 'beta [deg]' with '90', 'c [Angstrom]' with '5.2', 'gamma [deg]' with '120', a 'Crystal lattice' dropdown menu set to 'Orthorhombic', and a 'Space group' text box with '194_Mg'. At the bottom is a 'Save material file' button.

Enter Phase name, lattice constants, crystal structure, and space group. Save material file.

Click “Select phases” and select the saved material file.

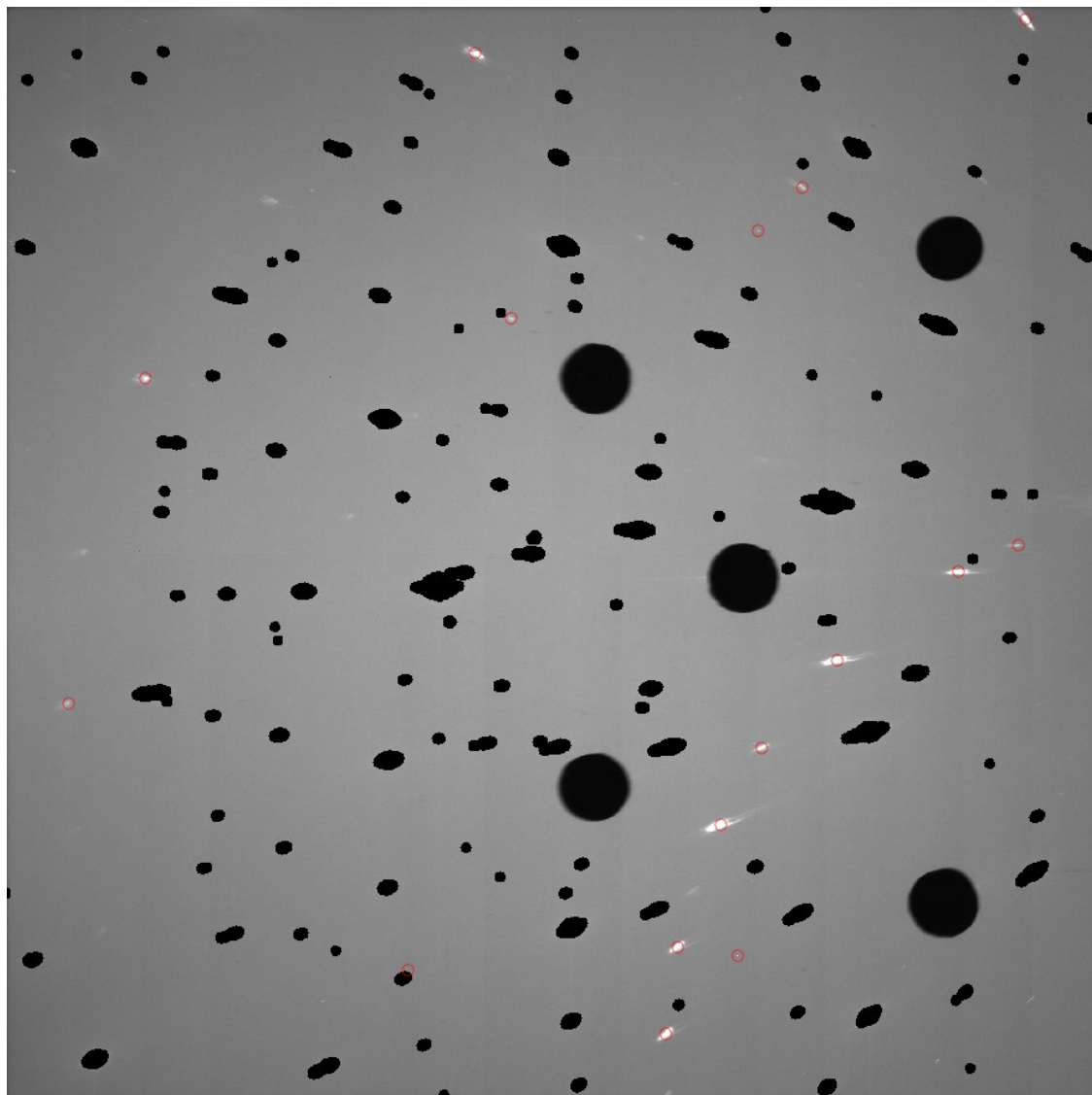
Check one phase from the list:



The image shows a window titled 'Phases to index'. It has two buttons at the top: 'Select phases' and 'Add a new phase'. Below these is a list of two items: 'Mg BCC.txt' with an unchecked checkbox and 'Mg HCP.txt' with a checked checkbox. Below the list is an empty rectangular box.

Auto spot search

Click **“Run auto spot search”** in attempt to automatically detect diffraction spots based on the brightness threshold. Detected spots will be indicated by red circles on the image:




Adjust threshold to find more or less spots.

Alternatively, spots can be added manually by left mouse click on the image.

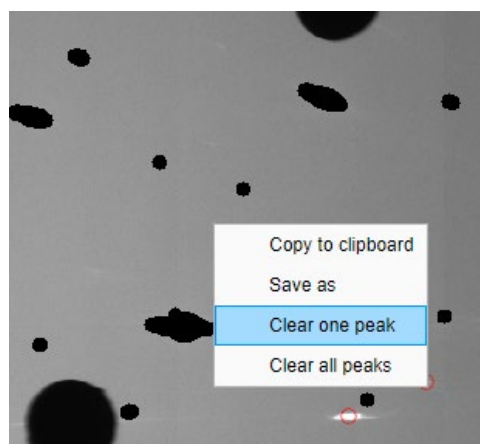
List of the selected spots can be observed in a tab **“Selected spots”**:

Selected spots

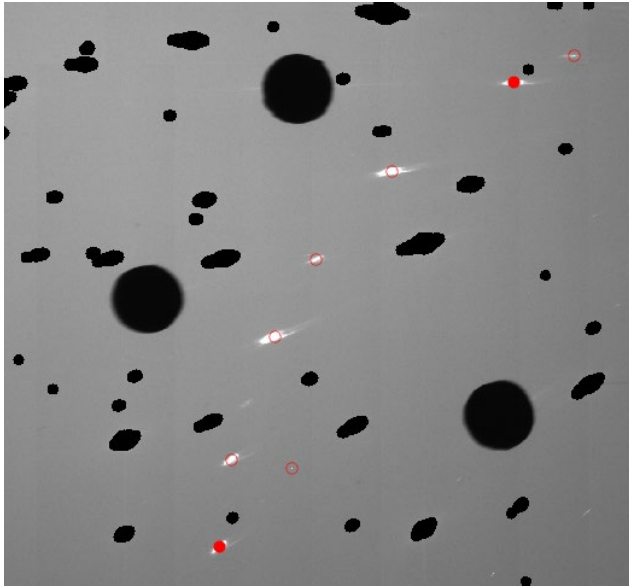
Peak number	Peak X	Peak Y	
1	121	1305	
2	266	700	
3	756	1803	
4	882	94	
5	948	588	
6	1237	1922	
7	1258	1760	
8	1339	1532	

Export spots

To remove a selected spot, right mouse click on the spot and select **“Clear one peak”**. To remove all selected spots, click **“Clear all peaks”**.



Once spots are selected, define two spots for the initial guess. This can be done by middle mouse click on the selected spots. Spots, selected for the initial guess will be highlighted by solid red circles:



On the left, check the box “Parallel computing” and click “Run indexing”

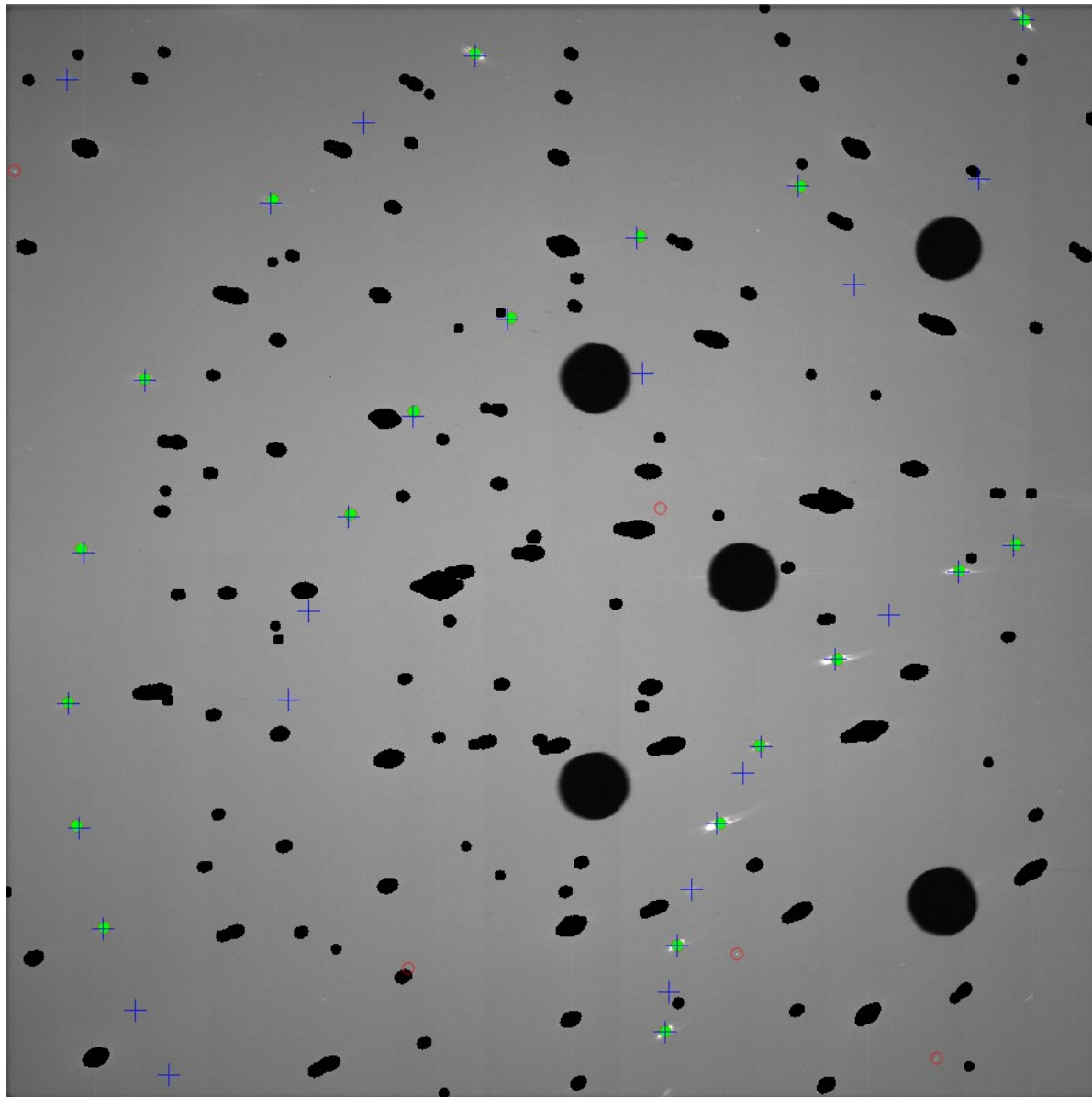
☒ Parallel computing

Run indexing

Solutions will be displayed in a table as soon as they are found:

Solutions			
Phase	HKL1	HKL2	Indexed spots
Mg HCP	2 1 1	1 0 -5	20

Click on the solution to display which spots were indexed in a solution (green solid color) and which ones are predicted (blue crosses):



Choose plotting options:

Min d-spacing, size, color, and shape of the plotted spots as well as hkl labels.

Plotting

d min [Å]

0 1 2 3 4 5

☒ Selected spots

Red Circle ☐ Filled

Size Edge Thickness

☒ Indexed spots

Green Circle ☒ Filled

Size Edge Thickness

☒ Predicted spots

Blue Cross ☐ Filled

Size Edge Thickness

☐ hkl labels

Blue Size

☐ Rotate lattice

1	1	0
-1	0	0
0	0	1

Most of the images in the UI can be copied to clipboard or saved upon right mouse click:

