Read the Docs Template Documentation

Release 0.2

Read the Docs

Nov 05, 2019

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EMSphInx is a collection of modules and programs that can be used to index a variety of diffraction patterns, ranging from EBSD to TKD, ECP, and x-ray Laue patterns. EMSphInx is currently a public beta; please report bugs to the issue tracker. If you use these programs for research, consider citing the corresponding papers:

- EBSD Indexing
- Pseudo-symmetry Prediction

CHAPTER 1

Financial Support

EMSphInx was developed with support from an ONR Vannevar Bush Faculty Fellowship grant, N00014-16-1-2821. The central indexing algorithm is covered by a provisional patent application.

CHAPTER 2

Installation

Nightly builds will be available soon for a variety of operating systems. Binaries are also available as assets for tagged releases .

EMSphInx requires CMake 3.14 or higher to build. All dependencies are downloaded and compiled as part of the build process by default. The easiest way to build a non-default version of EMSphInx is with the cmake gui or ccmake. If you are restricted to the command line and only need the default configuration you can build with the following sequence:

1. Download the source, create a build directory, and move into it

```
$ git clone https://github.com/EMsoft-org/EMSphInx
$ mkdir EMSphInxBuild
$ cd EMSphInxBuild
```

2. Run cmake and build

Run cmake and build. If you would like to build the GUIs you can optionally set the GUI CMake flag (EMSPHINX_BUILD_GUIS).

```
$ cmake ../EMSphInx
$ make -j
```

FFTW can compile SIMD instructions on some platforms even if they are not available on the current hardware. If you encounter illegal instructions at runtime try compiling with SIMD disabled (EMSPHINX_FFTW_SIMD). AVX2 instructions are disabled by default but can be enabled (EMSPHINX_FFTW_AVX2).

For example to build the GUI with no SIMD:

```
$ cmake ../EMSphInx -DEMSPHINX_BUILD_GUIS=ON -DEMSPHINX_FFTW_SIMD=OFF
$ make -j
```

CHAPTER 3

Contribute

- Issue Tracker: https://github.com/EMsoft-org/EMSphInx/issues
- Source Code: https://github.com/EMsoft-org/EMSphInx

CHAPTER 4

License

EMSphInx is distributed under a GPL2 license with several external dependencies. Please refer to the license page for details.

CHAPTER 5

Table of Contents

5.1 EMSphInxEBSD

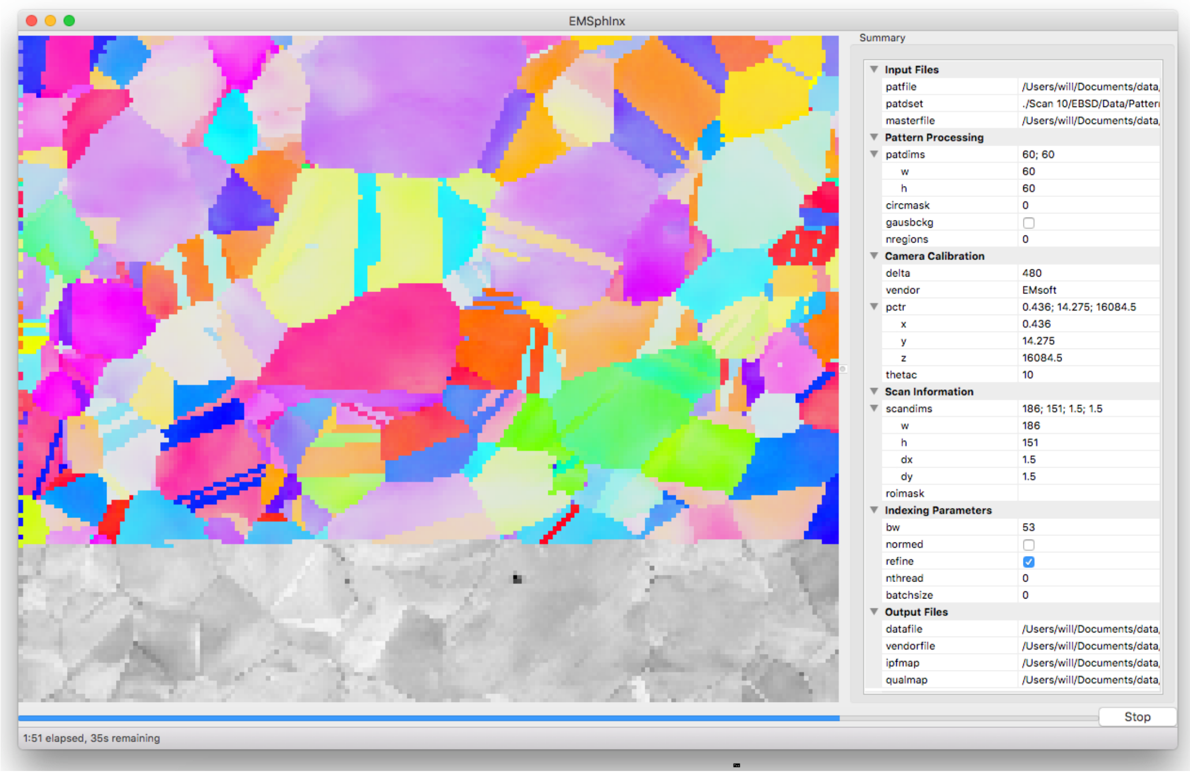
EMSphInxEBSD is a GUI for indexing EBSD patterns using spherical harmonics, part of the EMSphInx package.

5.1.1 Main Window

The main window consists of a menu bar (top), live indexing result (left), indexing parameters (right), and progress/status bar (bottom). To index an EBSD scan first specify the parameters by editing the summary panel directly, loading a namelist file, and/or using the wizard (Menu File Wizard). Once the parameters are specified hit the 'Start' button and indexing will begin.

Indexer initialization may take several minutes on the first run as Fourier transforms are being planned. To preplan DFTs use Menu Tools Build Wisdom.

The main window is split into 3 primary sections as seen in the screenshot below: live indexing result (left), *Parameter Summary Panel* (right), and status bar (bottom)



Menu Bar

File Menu

Item	Function
Open…	load indexing parameters from a namelist (.nml) file
Save…	save current indexing parameters from a namelist (.nml) file
Wizard…	build indexing parameters interactively using the wizard (the wizard will be prepopulated with current values if possible)

Tools Menu

Item	Function
Clear Wisdom	delete any accumulated wisdom, see **'FFTW Words of Wisdom'_** for details about FFT wisdom
Build Wisdom…	plan DFTs sizes needed for specified bandwidths
Import Wisdom…	load DFT plan wisdom from a file (adds to existing wisdom)
Export Wisdom…	export DFT plan wisdom to a file
Convert Master Pattern…	convert from EMsoft *.h5 master pattern format to EMSphInx *.sht format
Extract Master Projection…	extract a stereographic master pattern projection from a *.sht file

Please note that wisdom is hardware specific and for best performance shouldn't be shared between platforms.

Help Menu

Item	Function
About…	display information about this program
Citations…	display relevant citations - both for this program and for any currently selected master patterns
Help…	link to this documentation

Parameter Summary Panel

The parameter summary panel is split into 6 sections detailed below:

1. Input files - EBSD pattern source and simulated master pattern
2. Pattern Processing - pattern size and image preprocessing
3. Camera Calibration - detector geometry description
4. Scan Information - orientation map dimensions and region of interest
5. Indexing Parameters - spherical cross correlation and threading parameters
6. Output Files - locations to save indexing results

If you are uncomfortable filling parameters directly, use the wizard.

Input Files

Name	Type	Value
patfile	file	EBSD patterns to index (*.up1,* .up2, *.ebsp, or* .h5)
patdset	string	path to patterns within hdf5 file (ignored for other formats)
masterfile	file list	spherical master pattern files to index against (.sht), first file is phase 0 in output, second file is phase 1, etc.

Pattern Processing

Name	Type	Value
patdims.w	integer	width of detector in pixels
patdims.h	integer	height of detector in pixels
circmask	integer	circular mask radius (-1 for no mask, 0 for inscribed circle, >0 for radius in pixels)
gausbckg	boolean	should a 2D Gaussian background be subtracted from patterns
nregions	integer	number of tiles for adaptive histogram equalization (0 for no equalization)

Camera Calibration

Name	Type	Value
delta	real	detector pixel size in microns (i.e. patdims.w * delta is the width of the detector)
vendor	enum	pattern center convention (EMsoft, Bruker, EDAX, or Oxford)
pctr.x	real	pattern center calibration, see table below or refer to the EMsoft tutorial paper for details
pctr.y	real	
pctr.z	real	
theatc	real	camera elevation angle in degrees, refer to the EMsoft EBSD forward model paper for details

Pattern Center Conventions:

Name	EMsoft	Bruker	EDAX	Oxford
pctr.x	pixels	detector widths	detector widths	detector widths
pctr.y	pixels	detector widths	detector widths	detector heights
pctr.z	microns	detector heights	detector widths	detector widths
origin	center	top left	bottom left	bottom left

Scan Information

Name	Type	Value
scandims.w	integer	width of scan grid in pixels
scandims.h	integer	height of scan grid in pixels
scandims.dx	real	width of grid pixel in microns
scandims.dy	real	height of grid pixel in microns
roimask	string*	string representation of region of interest to index (or empty to index everything)

The ROI string is a series of (x,y) image coordinates (integer pixels) with 3 shapes defined:

1. Rectangle - first coordinate is origin, second coordinate is rectangle size
2. Ellipse - 'e' + bounding box as rectangle
3. Polygon - vertices in order (first/last point specified twice)

The region of interested can be inverted (the excluded region selected instead of the included region) by prepending the string with 'i'. Here are some ROI string examples:

- only points inside the rectangle with corners at (12, 34) and (56, 79) - "12, 34, 44, 45"
- the same rectangle specified as a polygon - "12, 34, 12, 79, 56, 79, 56, 34, 12, 34"
- only points outside the circle with radius 50 and center (60, 70) - "ie10, 20, 100, 100"

If you're uncomfortable manipulating the ROI string please use the wizard.

Indexing Parameters

Name	Type	Value
bw	integer	Bandwidth to index with - time scales as bw^3 * $\ln(bw^3)$ so the lowest tolerable value should be used. The Euler angle grid size is $(2 * bw - 1)^3$ so indexing is fastest when 2 * bw - 1 is a product of small primes. Slow sizes will be padded up to the nearest fast size so in practice most sizes are efficient. Here are some reasonable ideal sizes: • 53, 63, 68, 74 - fast but somewhat noise sensitive • 88, 95, 113, 123 - trade-off between noise tolerance and speed • 158, 172, 203, 221, 263 - maximum noise robustness but slow
normed	boolean	should normalized or unnormalized cross correlation be used for indexing - normalization is slightly slower but is suggested when pseudo-symmetry is anticipated or to index against multiple phases
refine	boolean	should newtons method refinement be used - slower but improves precision
nthread	integer	number of threads to index with (0 to determine from number of virtual cores) - performance peaks at ~1.5x the number of real cores
batchsize	integer	number of patterns to dispatch to a thread at once (0 to estimate a reasonable number based on bw) - extremely small values will incur additional threading overhead but large values make the 'stop' button take longer to work

Output Files

Name	Type	Value
datafile	file	location to write indexing results and meta data to (required)
vendorfile	file	optional location to write vendor file (.ang or .ctf)
ipfmap	file	optional location to write Z reference IPF map (.png)
qualmap	file	optional location to write (normalized) spherical cross correlation map (.png)

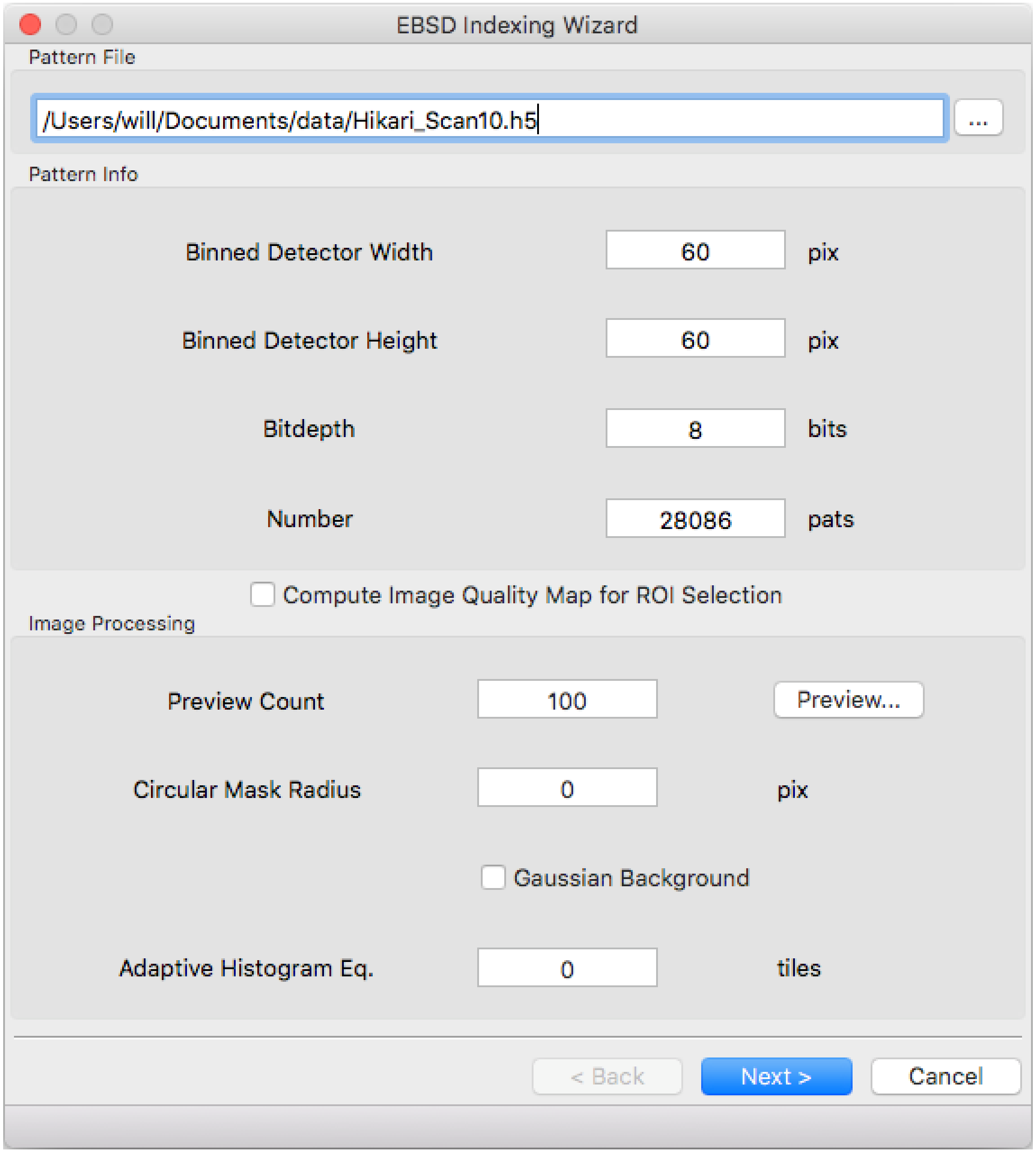
5.1.2 Parameter Wizard

The EBSD namelist generation wizard has 6 panels to interactively fill the required parameters for indexing:

1. Experimental Pattern Selection
2. Master Pattern Selection
3. Detector Geometry
4. Scan Geometry
5. Indexing Parameters
6. Summary

Any error messages are displayed in the status bar (bottom left)

Experimental Pattern Selection



Pattern File

File to read EBSD patterns from. HDF5 (.h5, .hdf, .hdf5), EDAX (.up1, .up2), Oxford (.ebsp), and EMsoft (.data) files are supported. The pattern dimensions, bitdepth, and number of patterns will be determined automatically for all files except EMsoft raw files. Additional meta data will be parsed depending on file type

- HDF5 EBSD scan files
- EDAX files when there is a .ang with the same path/name
- Oxford files when there is a .ctf with the same path/name

The following additional metadata will be read and prepopulated if possible:

- pattern center calibration
- detector tilt
- scan dimensions
- scan pixel size
- Pattern quality and indexing confidence maps (for ROI selection)

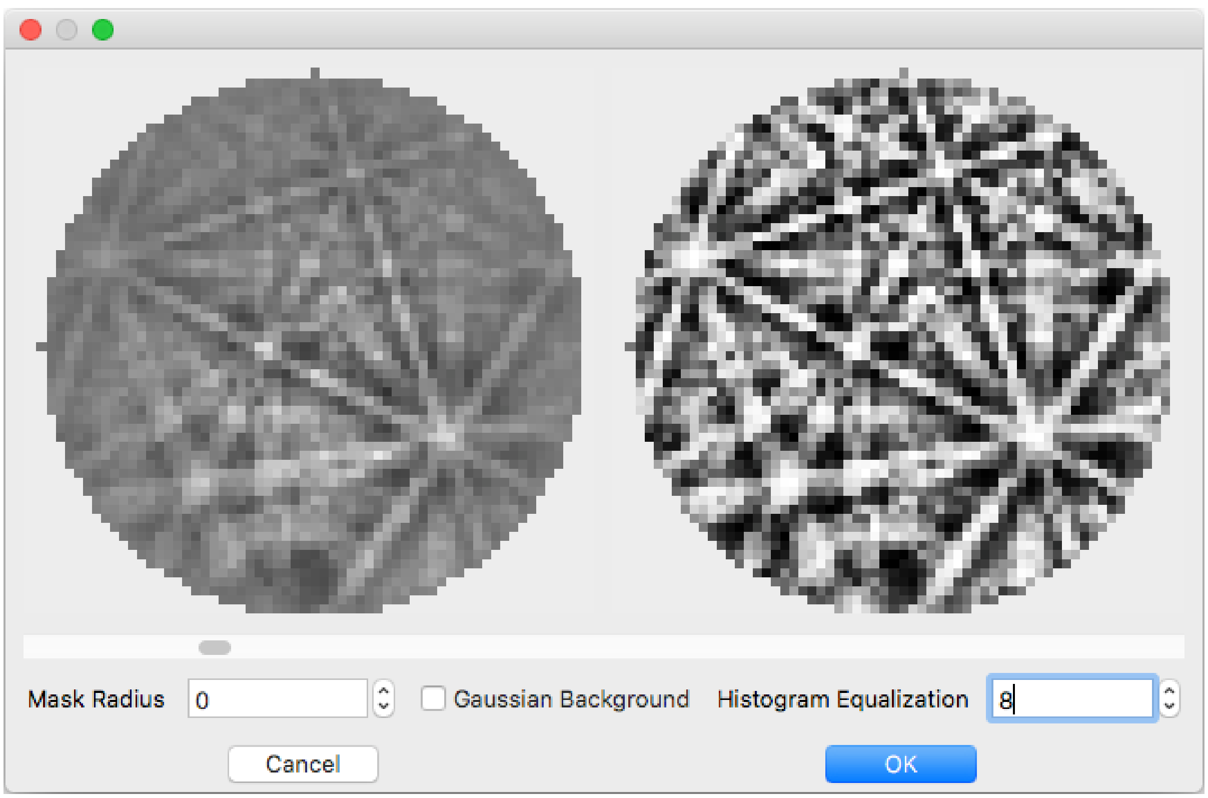
Pattern Info

Detector geometry will be automatically determined for most file formats. Raw binary files require specifying the pattern size.

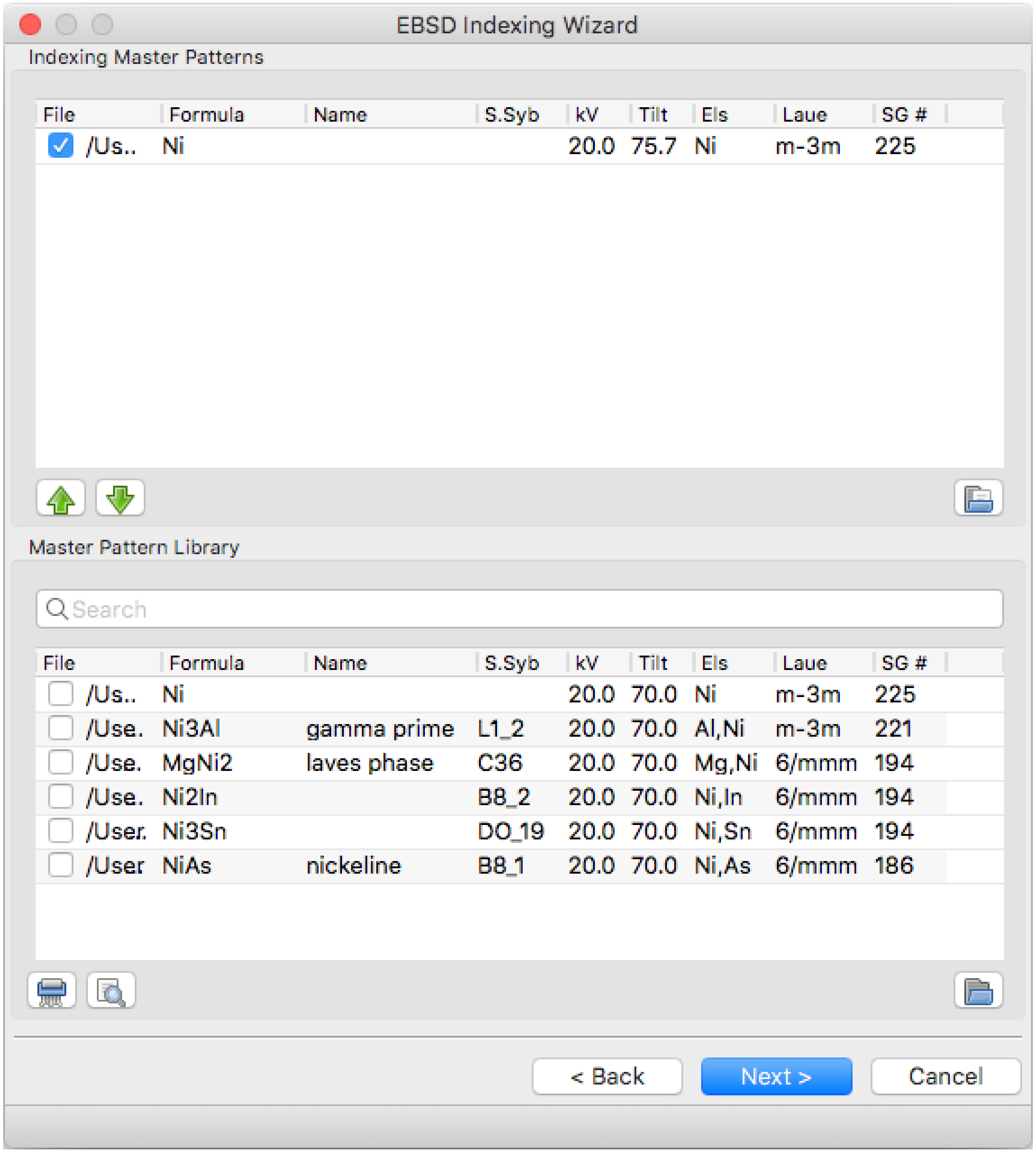
Image Processing

The easiest way to select parameters is with the 'Preview…' button. When the button is clicked 'Preview Count' evenly spaced patterns will be read from the file. The raw pattern is displayed on the left and the processed pattern on the right. Change which pattern is displayed with the scroll bar and adjust parameter values below. If the dialog is closed with the 'OK' button the current values will be populated into the wizard, otherwise they will be discarded.

If your pattern file doesn't have associated maps for ROI selection you can tick the 'Compute Image Quality Map for ROI Selection' box to calculate IQ during pattern loading. If the box is ticked a computed IQ map will be available on the 'Scan Geometry' page.



Master Pattern Selection



Indexing Master Patterns

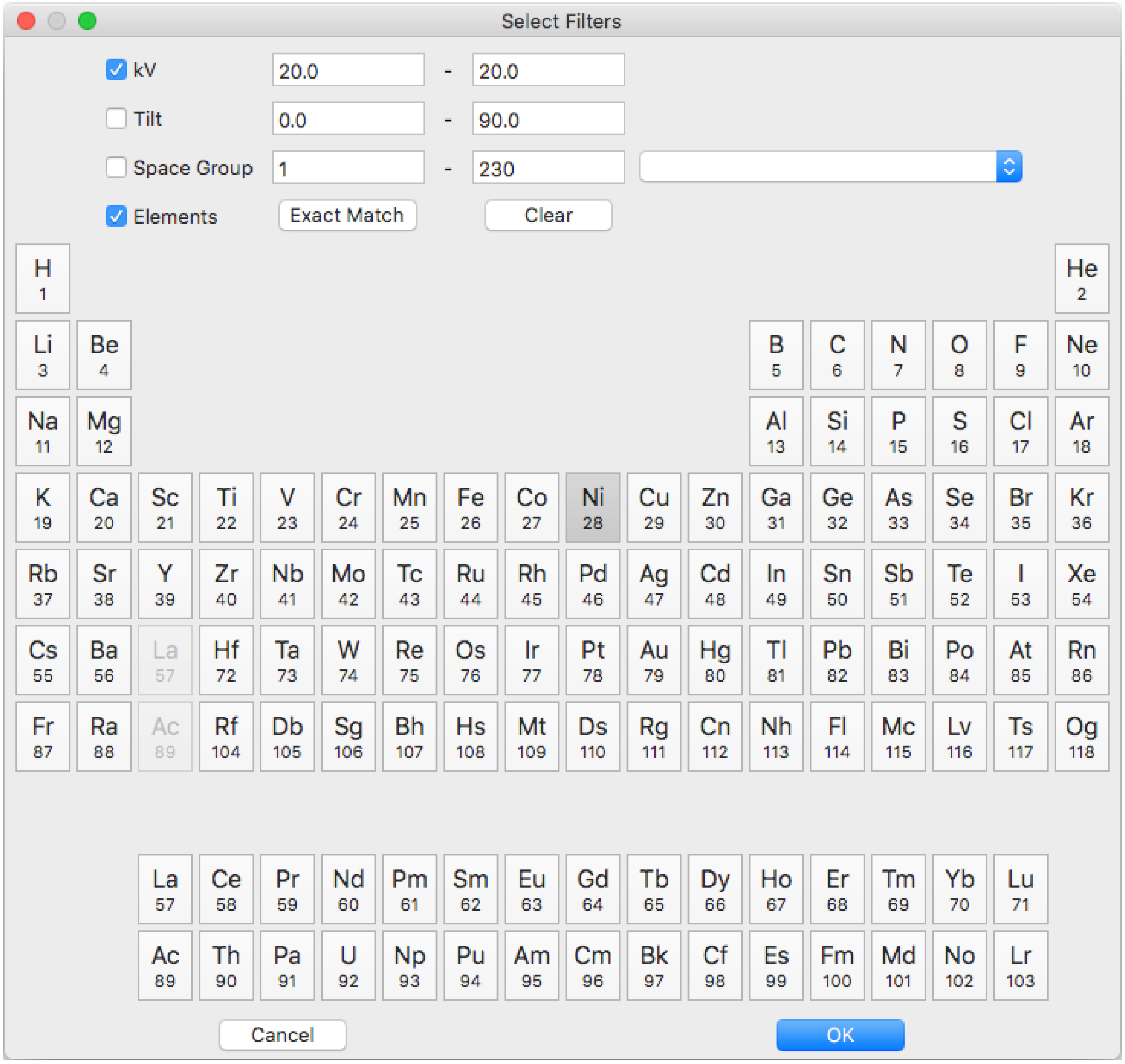
Spherical master patterns to index against. Multiple patterns can be selected for multi-phase indexing. The first pattern in the list is phase 0, the second phase 1, etc. Use the up/down arrow buttons (bottom left) to reorder patterns. Click the file brows button (bottom right) to browse for a single master pattern file (.sht) to add to the indexing list. Master patterns can be removed from the list by unticking the checkbox (OS X or Linux only) or double clicking.

Master Pattern Library

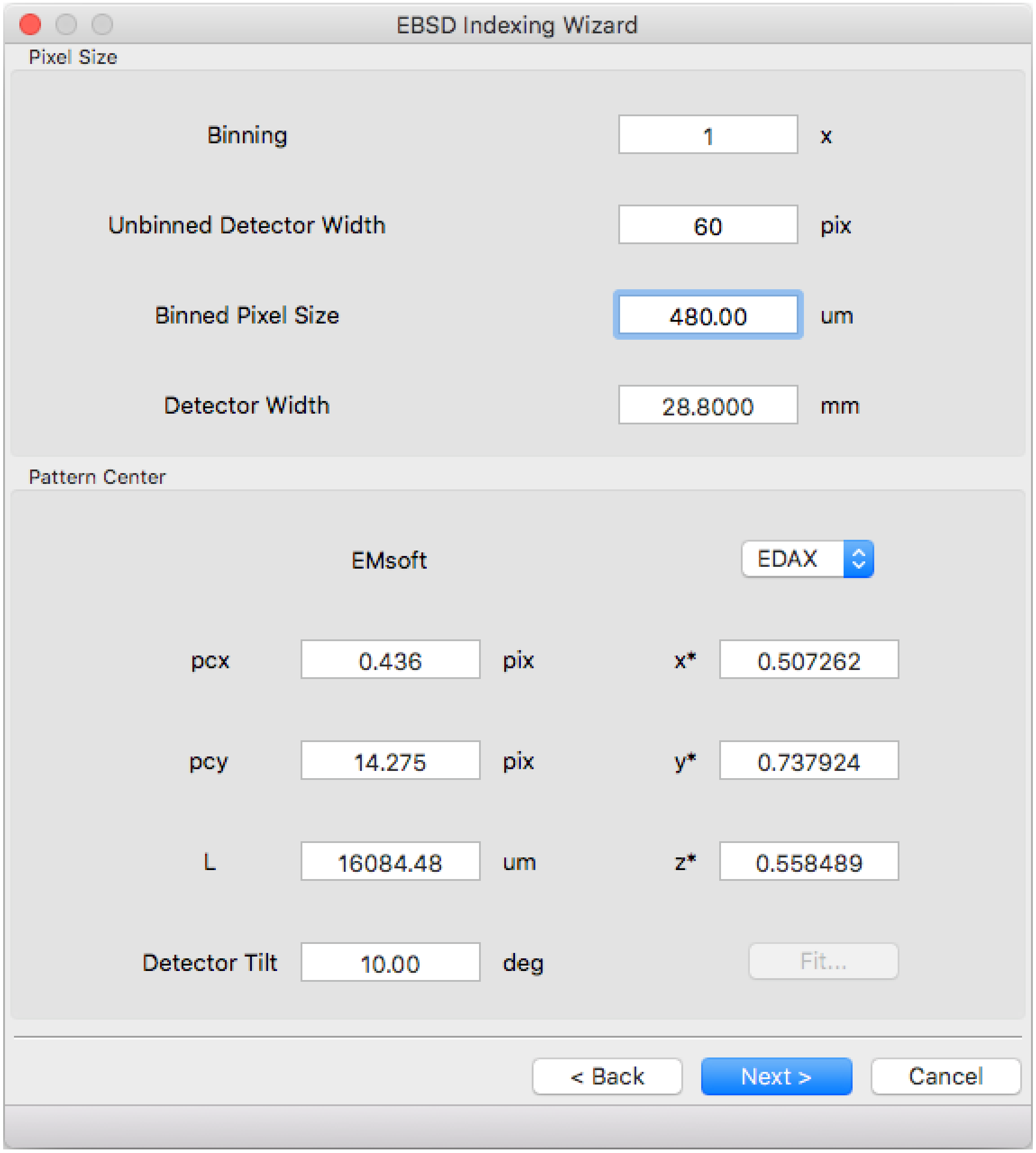
All previously used master patterns that aren't currently in the 'Indexing Master Patterns' box are listed here. Master patterns can be sorted by clicking on the column headers:

- File - full path the master pattern file
- Formula - material formula string
- Name - material/phase name
- S.Syb - structure symbol
- kV - accelerating voltage
- Tilt - sample tilt (degrees)
- Laue - crystal Laue group
- SG# - space group number (effective for overlap patterns)

Known master patterns can be permanently removed from the list by selecting and then pressing the delete button (bottom left). Displayed master patterns can be filtered by file, formula, name, or s.syb with the search bar (top). Use the search button (bottom left) to filter by kV, Tilt, SG#, and/or composition. All master pattern files in a folder (recursive) can be added with the directory browse button (bottom right). Master patterns can be move to the indexing list by ticking the checkbox (OS X or Linux only) or double clicking.


Select Filters
kV 20.0 - 20.0
Tilt 0.0 - 90.0
Space Group 1 - 230
Elements
Exact Match
Clear
H 1
He 2
Li 3 Be 4 B 5 C 6 N 7 O 8 F 9 Ne 10
Na 11 Mg 12 Al 13 Si 14 P 15 S 16 Cl 17 Ar 18
K 19 Ca 20 Sc 21 Ti 22 V 23 Cr 24 Mn 25 Fe 26 Co 27 Ni 28 Cu 29 Zn 30 Ga 31 Ge 32 As 33 Se 34 Br 35 Kr 36
Rb 37 Sr 38 Y 39 Zr 40 Nb 41 Mo 42 Tc 43 Ru 44 Rh 45 Pd 46 Ag 47 Cd 48 In 49 Sn 50 Sb 51 Te 52 I 53 Xe 54
Cs 55 Ba 56 La 57 Hf 72 Ta 73 W 74 Re 75 Os 76 Ir 77 Pt 78 Au 79 Hg 80 Tl 81 Pb 82 Bi 83 Po 84 At 85 Rn 86
Fr 87 Ra 88 Ac 89 Rf 104 Db 105 Sg 106 Bh 107 Hs 108 Mt 109 Ds 110 Rg 111 Cn 112 Nh 113 Fl 114 Mc 115 Lv 116 Ts 117 Og 118
La 57 Ce 58 Pr 59 Nd 60 Pm 61 Sm 62 Eu 63 Gd 64 Tb 65 Dy 66 Ho 67 Er 68 Tm 69 Yb 70 Lu 71
Ac 89 Th 90 Pa 91 U 92 Np 93 Pu 94 Am 95 Cm 96 Bk 97 Cf 98 Es 99 Fm 100 Md 101 No 102 Lr 103
Cancel
OK

Detector Geometry



Pixel Size

Indexing requires the effective pixel size of the EBSD patterns in microns. Most scintillator based detectors have a pixel size of 50-100 microns. However if the detector is binned the effective pixel size increases by the binning factor. The unbinned detector width is read only and specified in pixels (it is the size from the Experimental Pattern Selection page). Consider a 640x480 detector with 50 micron pixels used to collect patterns with 4x4 binning:

- The pattern size is 160x120
- The effective pixel size is 200 microns (50 * 4)

- The detector width is 32 mm or 32000 microns (640 * 50 == 160 * 200)

'Binned Pixel Size' is the effective pixel size assuming the patterns were collected using 'Binning' x 'Binning' camera binning. Assuming that 'Binning', 'Binned Pixel Size', and 'Detector Width' are specified, then changing one will update the others accordingly:

- If 'Binning' is changed 'Binned Pixel Size' will be updated to keep 'Detector Width' constant
- If 'Binned Pixel Size' is changed 'Detector Width' will be updated using the current 'Binning'
- If 'Detector Width' is changed 'Binned Pixel Size' will be updated using the current 'Binning'

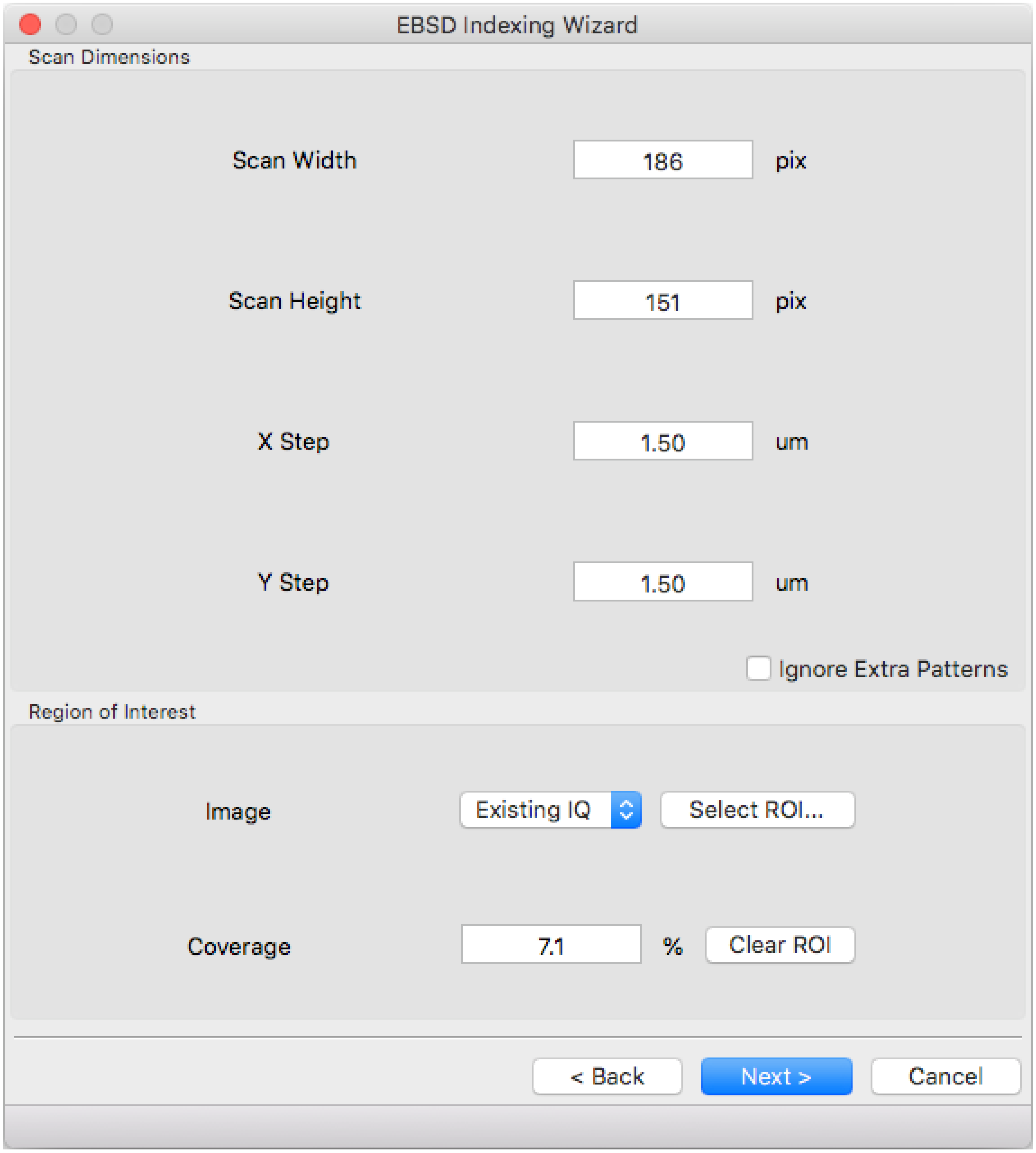
For the above example, the following combinations are all valid. Binning == 1 uses the effective experimental parameters, binning == 4 allows specifying the true pixel size, and other values are mathematically equivalent:

Binning	Unbinned Detector Width	Binned Pixel Size	Detector Width
1	160 pixels	200 um	32 mm
2	320 pixels	100 um	32 mm
4	640 pixels	50 um	32 mm
8	1280 pixels	25 um	32 mm

Pattern Center

The EMsoft pattern center is computed from the normalized pattern center using the binned pattern dimensions and pixel size. If the vendor dropdown is changed the normalized pattern center will be computed from the EMsoft pattern center using the current pixel size. The "Fit…" button is currently disabled but will be used for pattern center refinement in the future. Please refer to the EMsoft tutorial paper for details on pattern center and the EMsoft EBSD forward model paper details on the geometric model.

Scan Geometry



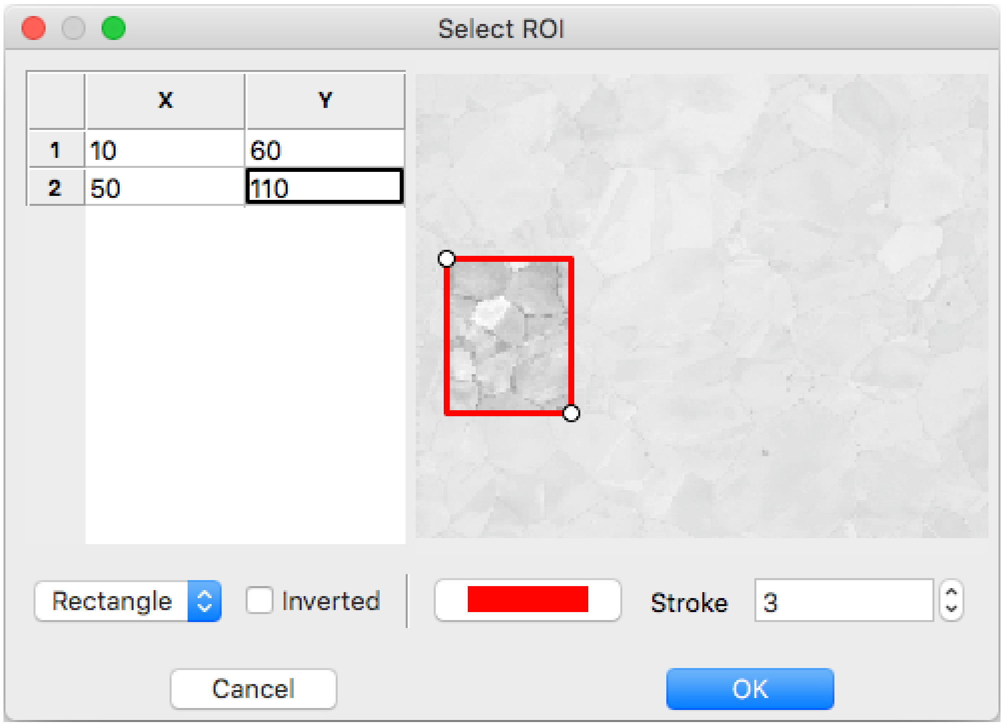
Scan Dimensions

Specify the number or columns / rows in the EBSD map scan grid and the grid pixel size in microns

Region of Interest

A region of interest (ROI) can be used to restrict indexing to a subset of the scan. ROI building requires a grayscale map either computed or loaded during experimental pattern selection. The percentage of pixel contained in the ROI is displayed in the coverage box and the ROI can be removed (index everything) with the clear button. To draw an ROI interactively click the 'Select ROI. . . ' button.

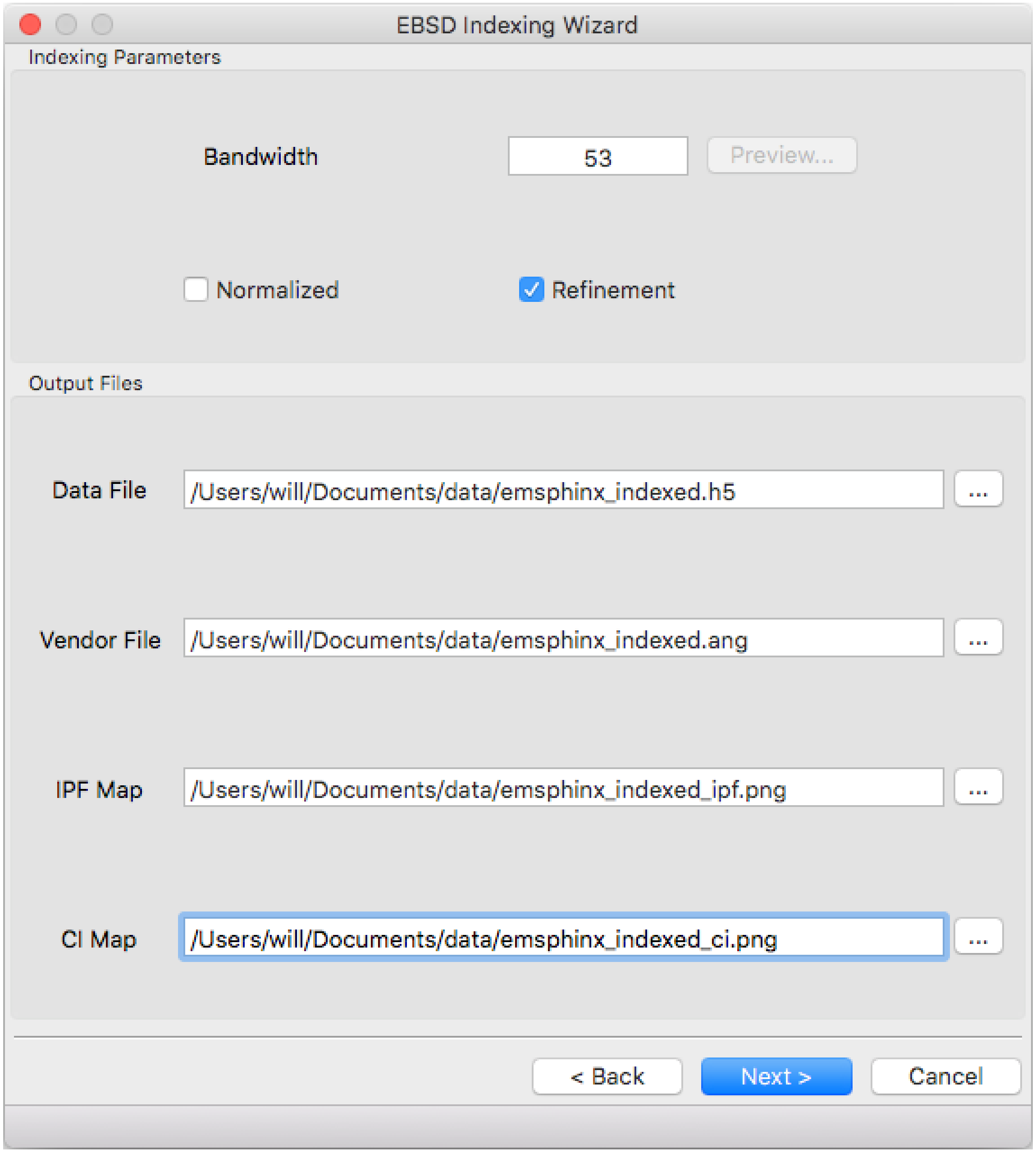
ROI Drawing Dialog



Select the ROI shape from the dropdown and draw a region accordingly. Pixels to index are unmodified and pixels to skip are grayed. Tick the inverted box to draw an exclusion region instead of an inclusion region. An existing ROI can be adjusted by clicking + dragging on a handle to change the shape or inside the selection to translate. If fine control on ROI positioning is needed the coordinates can be edited directly on the left.

- Rectangle - click on origin + drag to extend (hold shift during drag for square)
- Ellipse - click on bounding box origin + drag to extend (hold shift during drag for circle)
- Polygon - click to start
  - During construction
    - click to start / add a new point
    - hold shift to snap line to horizontal or vertical
    - press delete to remove the most recent point
    - right click to close shape
  - After construction
    - right click on a point to remove it
    - double click on a point to duplicate it (inserted after point)

Indexing Parameters



Specify the bandwidth, if normalize/unnormalized cross correlation should be used, and if newton's method based refinement should be used.

Bandwidth

Indexing bandwidth, refer to the Indexing Parameters section of the *Parameter Summary Panel* documentation for details.

Normalization

Using normalized spherical cross correlation is slightly slower but is suggested when pseudo-symmetry is anticipated or to index against multiple phases.

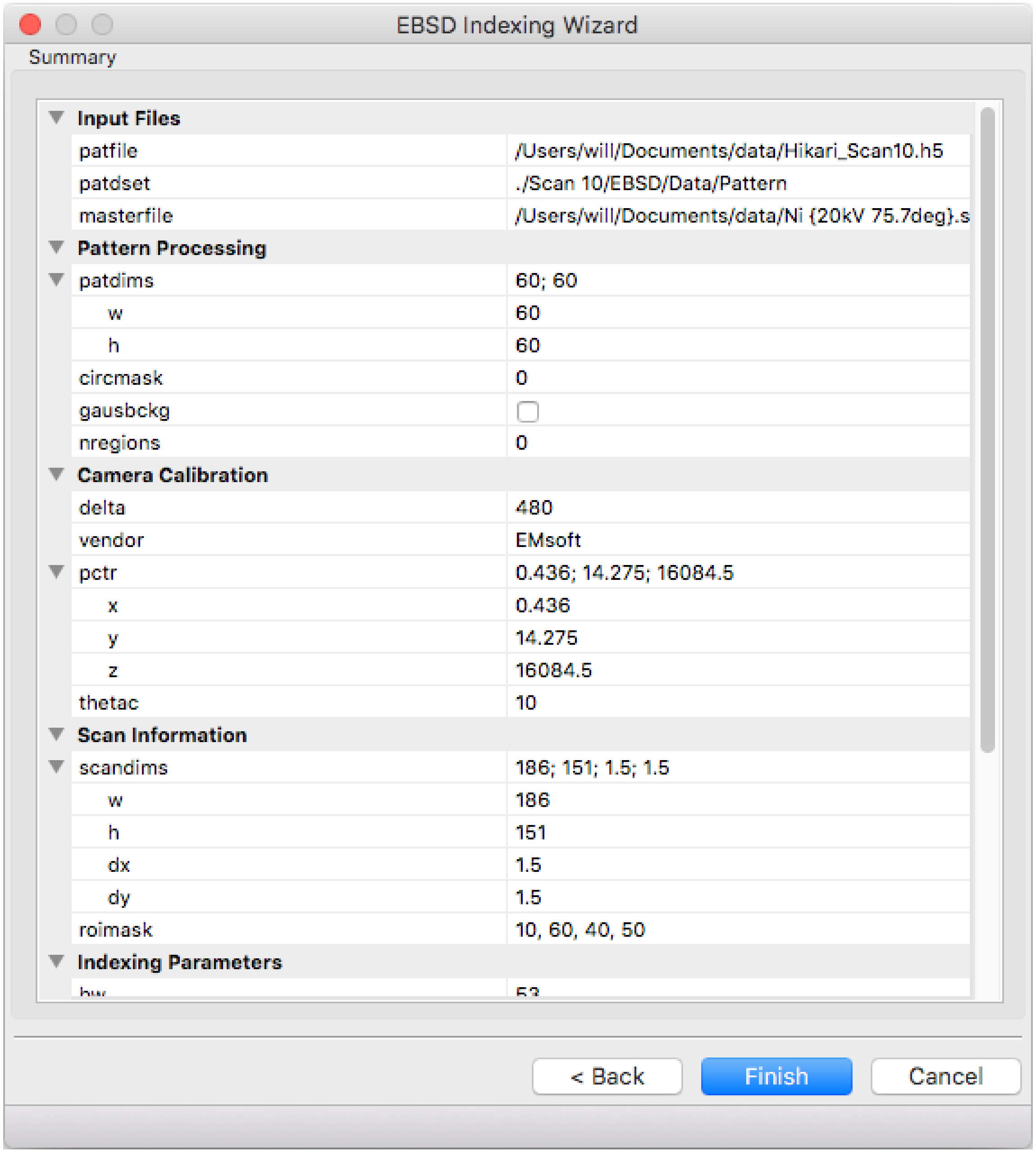
Refinement

Newtons method refinement add some overhead but gives maximum orientation precision. If refinement is unticked then a sub-pixel maximum will be interpolated from the 3x3x3 box surrounding the maximum in the Euler angle grid.

Output Files

An output data file is required and contains the indexing results as well as all parameter metadata. A vendor file (ang or ctf) can be optionally generated to help import results into other software packages. Finally IPF (z reference) and spherical cross correlation maps (png) can be optionally generated.

Summary



A read only summary of the generated parameters is displayed. Refer to the *Parameter Summary Panel* for details.

5.1.3 Example Data

The full 10 scan sequence used in the indexing paper can be downloaded here. The entire sequence is ~600 MB, a smaller file (~80 MB) containing only scan 10 is also available. A nickel master pattern corresponding to the scan conditions is in the github repo

Reasonable selections to walk through wizard for this dataset (only non-default values listed):

1. Experimental Pattern Selection - Pattern File: HikariNiSequence.h5 - Scan 10

2. Master Pattern Selection
    - Indexing Master Patterns: Ni {20kV 75.7deg}.sht
3. Detector Geometry
    - Binning: 1
    - Binned Pixel Size: 475
4. Scan Geometry (no changes)
5. Indexing Parameters
    - Bandwidth: 53
    - Refinement:
6. Summary (read only)

5.2 License

EMSphInx source files are distributed under GNU General Public License v2.0 (GPL2), see the license pages for details. EMSphInx includes source from several other projects:

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    - © 2003, 2007-11 Matteo Frigo, Massachusetts Institute of Technology
- several crystallographic and utility libraries - GPL2 licence
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CHAPTER 6

Indices and tables

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- modindex
- search