LaueTools Documentation

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CONTENTS

1 Introduction **1**
- 1.1 Tools . . . 1
- 1.2 Developers . . . 1
- 1.3 Browse Modules and Functions . . . 1

2 Installation **3**
- 2.1 How to Get LaueTools code . . . 3
- 2.2 Build LaueTools Documentation . . . 3

3 Getting started **5**
- 3.1 Launch Graphical User Interfaces of LaueTools . . . 5

4 Conventions **7**
- 4.1 Mathematics and Conventions . . . 7

5 Graphical User Interfaces **9**
- 5.1 Interactive Graphical User Interfaces . . . 9
- 5.2 Batch Processing Graphical User Interfaces . . . 9

6 Tutorials **11**
- 6.1 Basics of Laue Pattern peak search and Unit cell Refinement . . . 11
- 6.2 Indexation of spots data set. . . . 33

7 LaueTools Modules **53**
- 7.1 Browse Modules and Functions . . . 53
- 7.2 Modules for Laue Pattern Simulation . . . 53
- 7.3 Modules for Digital Image processing, Peak Search & Fitting . . . 77
- 7.4 Modules for Laue Pattern Indexation . . . 103
- 7.5 Modules for Crystal unit cell refinement . . . 103
- 7.6 Modules for batch processing . . . 103

Python Module Index **105**

Index **107**

CHAPTER

ONE

INTRODUCTION

LaueTools is a **python** written package aiming at analysing from 1 to few 10000s microdiffraction Laue patterns coming from synchrotron CRG-IF BM32 beamline at ESRF.

With pip installer, it is now relatively easy to install LaueTools and put hands immediately on data. See *Installation* page.

1.1 Tools

LaueTools has got :

- Modules to be imported in your own scripts like any **scientific library**.
- LaueTools has got several *Graphical User Interfaces* to interact graphically with data so that to accelerate the design of future scripts and to set the most finely of parameters for batch processing.
- **Notebooks** to guide the typical way you can handle the data (visualisation, selection, analysis, post processing)

1.2 Developers

Developers are welcome to improve the code readability and to add new functionalities. Please contact us.

1.3 Browse Modules and Functions

- genindex
- modindex

CHAPTER

TWO

INSTALLATION

Some dependencies are rather usual (numpy, scipy, matplotlib) while others are more uncommon but very useful (fabio, networkx).

GUIs are based on wxpython graphical libraries which can be tricky to install (Sorry. We are working on it).

2.1 How to Get LaueTools code

- Download the very last version of the code at **gitlab.esrf.fr** (but you are also welcome to fork this project):

  https://gitlab.esrf.fr/micha/lauetools

- or Download last (or older releases) on **pypi** by means of pip

  https://pypi.org/project/LaueTools/

  if pip is installed:

```
pip install lauetools
```

2.2 Build LaueTools Documentation

Documentation can be generated, by installing sphinx and a cool html theme:

```
pip install sphinx

pip install sphinx-rtd-theme
```

You may need rinohtype:

```
pip install RinohType
```

Then from /LaueTools/Documentation folder which contains *Makefile* and 2 folders *build* and *source*, build the documentation

```
make html
```

Files in html format will be browsed in /build/html folder with any web navigator. You can start with index.html.

CHAPTER

THREE

GETTING STARTED

3.1 Launch Graphical User Interfaces of LaueTools

- start Lauetools GUIs from command line :

To deal with relative import, the package name 'LaueTools' must be specified to the python interpreter as following

Examples:

- python -m LaueTools.LaueToolsGUI
- python -m LaueTools.LaueSimulatorGUI
- python -m LaueTools.PeaksearchGUI

The first main GUI, LaueToolsGUI can open also the two last GUIs (LaueSimulatorGUI, PeaksearchGUI)

There are additional basic GUIs for batch processing located in FileSeries folder:

- python -m LaueTools.FileSeries.Peak_Search
- python -m LaueTools.FileSeries.Index_Refine
- python -m LaueTools.FileSeries.Build_summary
- python -m LaueTools.FileSeries.Plot_Maps2
- within interactive python (say, ipython -i), GUI can be started thanks to a start() function:
  - In [1] : import LaueTools.LaueToolsGUI as LTGUI
  - In [2] : LTGUI.start()

Note: in the LaueTools folder :

- neither > python LaueToolsGUI
- nor in >ipython -i : > run LaueToolsGUI will work...

3.1.1 Use LaueTools module as a library

With pip installation, LaueTools package will be included to python packages. Therefore any module will be callable as the following:

-In [1] : import LaueTools.readmccd as rmccd

-In [2] : rmccd.readCCDimage('myimage.tif')

In jupyter-notebook, it is also simple in the same manner:

```
In [2]: import LaueTools.CrystalParameters as CP

...

In [5]: Gstar=CP.Gstar_from_directlatticeparams(5.65,5.65,5.65,90,90,90)

In [7]: CP.DSpacing([1,1,1],Gstar)
Out[7]: 3.2620290209213856

In [8]: import math
        5.65/math.sqrt(3)
Out[8]: 3.262029020921386
```

CHAPTER

FOUR

CONVENTIONS

4.1 Mathematics and Conventions

CHAPTER

FIVE

GRAPHICAL USER INTERFACES

LaueTools provides two types of GUI:

- GUI with graphical interaction when handling data
- GUI used as input file parameters for batch processing

5.1 Interactive Graphical User Interfaces

The main steps of analysis are Laue peaks search, Laue Pattern indexation and unit Cell Refinement. Detector geometry calibration (DetectorCalibrationBoard) and Laue Pattern of Polycrystals (LaueSimulatorGUI) are also available.

5.1.1 Peak Search (PeaksearchGUI)

5.1.2 Indexation (LaueToolsGUI)

5.1.3 Crystal unit cell refinement (LaueToolsGUI)

5.1.4 Detector Geometry Calibration (DetectorCalibrationBoard)

5.1.5 Laue pattern simulation of assembly of crystals (LaueSimulatorGUI)

5.2 Batch Processing Graphical User Interfaces

CHAPTER

SIX

TUTORIALS

6.1 Basics of Laue Pattern peak search and Unit cell Refinement

6.1.1 This Notebook is a part of Tutorials on LaueTools Suite.

Author: J.-S. Micha

Last Revision: August 2019

tested with python3

Objectives

- Load and display Laue pattern images
- Perform a Peak Search
- Perform the indexation of a Laue spots list
- Perform the crystal orientation and unit cell refinement

Setting absolute path to LaueTools Modules if Lauetools has not been installed with pip. It is assumed that this notebook is located in a subfolder (normally Notebooks)

```
LaueToolsCode_Folder = '..'
import sys,os
abspathLaueTools =os.path.abspath(LaueToolsCode_Folder)
print('abspathLaueTools',abspathLaueTools)
sys.path.append(LaueToolsCode_Folder)
```

```
abspathLaueTools /home/micha/LaueToolsPy3/LaueTools
```

```
import LaueTools
LaueTools.__file__
```

```
'/home/micha/LaueToolsPy3/LaueTools/__init__.py'
```

```
#%matplotlib inline
%matplotlib notebook

import time,copy,os

# Third party modules
import matplotlib     # graphs and plots
```

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```
import matplotlib.pyplot as plt
import numpy as np     # numerical arrays

# LaueTools modules

import LaueTools.IOLaueTools as IOLT    # read and write ASCII file  (IO)
import LaueTools.readmccd as RMCCD # read CCD and detector binary file, PeakSearch␣
↪methods
```

```
LaueToolsProjectFolder /home/micha/LaueToolsPy3/LaueTools
```

```
/home/micha/anaconda3/lib/python3.6/site-packages/h5py/__init__.py:36:␣
↪FutureWarning: Conversion of the second argument of issubdtype from float␣
↪to np.floating is deprecated. In future, it will be treated as np.float64␣
↪== np.dtype(float).type.
  from .conv import register_converters as _register_converters
```

```
module Image / PIL is not installed
Cython compiled module 'gaussian2D' for fast computation is not installed!
module Image / PIL is not installed
```

Considering single image analysis (that belong to the LaueTools distribution)

```
t0 = time.time()
LaueToolsExamplesFolder = os.path.join(LaueToolsCode_Folder,'Examples')

imageindex = None
imagefolder =os.path.join(LaueToolsCode_Folder,'LaueImages')
imagefilename = 'Ge_blanc_0000.mccd'

#imagefolder =os.path.join(LaueToolsCode_Folder,'LaueImages')
#imagefilename = 'CdTe_I999_03Jul06_0200.mccd'
```

Considering analysis of one image in dataset

For information: select image file of interest, in case of set of images with index. Then, splitting imagefilename allows to loop over images: prefix+index.extension

```
%%script false
# just to show (cell not executed)

imagefolder ='/home/micha/LaueProjects/VO2/ToScript/Data_VO2'

prefixfilename= 'CT30_'
imageindex=20

imagefilename = prefixfilename+'%04d.mccd'%imageindex
print("imagefilename :",imagefilename)
# you should see: imagefilename : CT30_0020.mccd
```

Read image file, get data and display it

Function `readCCDimage()` returns `dataimage` as a 2D numpy array with the proper dimensions and orientation given by `framedim` and the geometrical transformations labelled by `fliprot`

```
print('Displaying %s\n'%imagefilename)
dataimage, framedim, fliprot = RMCCD.readCCDimage(imagefilename,dirname=imagefolder,
↪CCDLabel='MARCCD165')
fullpathimagefile= os.path.join(imagefolder,imagefilename)

fig, ax = plt.subplots(figsize=(4,4))

ax.imshow(dataimage,vmin=0,vmax=2000)
ax.set_title('%s'%imagefilename)
```

```
Displaying Ge_blanc_0000.mccd

nb elements 4194304
framedim (2048, 2048)
framedim nb of elements 4194304
```

```
<IPython.core.display.Javascript object>
```

```
Text(0.5,1,'Ge_blanc_0000.mccd')
```

peaksearch is performed in two main steps: - 1) blobs or local maxima finder - 2) for blob, refinement starting from blob average center.

For the first step, `readCCDimage()` is called to obtain raw data if no different data array is provided with the argument `Data_for_localMaxima` (set to `None` by default). After second step, Peaksearch results can be purged from peaks already present in a file as an optional argument `Remove_BlackListedPeaks_fromfile`.

```
import os
ti1= time.time()

#blacklistedpeaksfile=os.path.join(folder,'Blacklist.dat')
blacklistedpeaksfile = None

res=RMCCD.PeakSearch(fullpathimagefile,CCDLabel='MARCCD165',
                     return_histo=0,local_maxima_search_method=0,
                     IntensityThreshold=200,
                     boxsize=5,
                     fit_peaks_gaussian=1,
                     FitPixelDev=10,
                     Data_for_localMaxima=None,#newdataimage,
                     Remove_BlackListedPeaks_fromfile=blacklistedpeaksfile)
tps =time.time()
print("peak search time",tps-ti1)
```

```
CCDLabel:  MARCCD165
nb of pixels (4194304,)
nb elements 4194304
framedim (2048, 2048)
framedim nb of elements 4194304
image from filename ../LaueImages/Ge_blanc_0000.mccd read!
Read Image. Execution time : 0.006 seconds
Data.shape for local maxima (2048, 2048)
Using simple intensity thresholding to detect local maxima (method 1/3)
len(peaklist) 82
Local maxima search. Execution time : 0.336 seconds
Keep 82 from 82 initial peaks (ready for peak positions and shape fitting)
```

```
*************
82 local maxima found

 Fitting of each local maxima

addImax False
nb elements 4194304
framedim (2048, 2048)
framedim nb of elements 4194304
framedim in readoneimage_manycrops (2048, 2048)
fitting time for 82 peaks is : 0.2039
nb of results:  82
After fitting, 0/82 peaks have been rejected
 due to (final - initial position)> FitPixelDev = 10
0 spots have been rejected
 due to negative baseline
0 spots have been rejected
 due to much intensity
0 spots have been rejected
 due to weak intensity
0 spots have been rejected
 due to small peak size
0 spots have been rejected
 due to large peak size
ToTake {0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19,␣
 ↪20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38,␣
 ↪39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57,␣
 ↪58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76,␣
 ↪77, 78, 79, 80, 81}
len(ToTake) 82

82 fitted peak(s)

Removing duplicates from fit

82 peaks found after removing duplicates (minimum intermaxima distance = 5)
peak search time 0.5514366626739502
```

Spots properties:

peak_X, peak_Y, peak_I, peak_fwaxmaj, peak_fwaxmin, peak_inclination, Xdev, Ydev, peak_bkg, Ipixmax,

Spots are sorted by intensity (according to the 2D gaussian fit)

```
peaklist=res[0]
print('Digital Spots properties for the 5 most intense spots')
print(peaklist[:6])
```

```
Digital Spots properties for the 5 most intense spots
[[ 6.231334887002143e+02  1.657728161614024e+03  2.979937967247360e+04
   8.515577956136006e-01  7.511212178165599e-01  1.820409415704489e+01
   1.334887002143432e-01 -2.718383859764799e-01  2.966046444454810e+02
   2.000000000000000e+02]
 [ 1.244326205473488e+03  1.662150473603958e+03  2.242563070589073e+04
```

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```
   6.977180389301006e-01  6.390759549880105e-01  1.293529253564775e+02
   3.262054734875619e-01  1.504736039580621e-01  1.998717405717028e+02
   2.000000000000000e+02]
 [ 9.330365915823824e+02  1.215440948340315e+03  2.219753607623998e+04
   7.846021988134166e-01  7.862341648303387e-01  3.246533552343026e+02
   3.659158238235705e-02  4.409483403153445e-01  2.110241433113940e+02
   2.000000000000000e+02]
 [ 5.852254505694141e+02  5.887990375606668e+02  9.528825561251553e+03
   7.791458064142315e-01  7.399755695034808e-01  1.068330480796285e+02
   2.254505694140789e-01 -2.009624393332388e-01  1.501265419627265e+02
   2.000000000000000e+02]
 [ 1.276607259246803e+03  6.002998208781320e+02  9.153971543092421e+03
   8.153699693677648e-01  8.035243472697837e-01  8.044575533084571e+01
  -3.927407531973586e-01  2.998208781319818e-01  1.324821469609317e+02
   2.000000000000000e+02]
 [ 9.326643784727646e+02  7.500763813513167e+02  6.940078500922347e+03
   7.065049204848781e-01  7.482895847319173e-01  8.063512928783894e+00
  -3.356215272353893e-01  7.638135131674062e-02  1.317606341369902e+02
   2.000000000000000e+02]]
```

```
print('X, Y pixel refinement positions for the first 5 spots')
peaklist[:5,:2]
```

```
X, Y pixel refinement positions for the first 5 spots
```

```
array([[ 623.1334887002143, 1657.7281616140235],
       [1244.3262054734876, 1662.150473603958 ],
       [ 933.0365915823824, 1215.4409483403153],
       [ 585.2254505694141,  588.7990375606668],
       [1276.6072592468026,  600.299820878132 ]])
```

add markers to image

```
if len(peaklist)<=1: raise ValueError

#datatoplot=newdataimage
datatoplot = dataimage

fig, ax = plt.subplots()
ax.imshow(datatoplot,vmin=0,vmax=1000,cmap='hot')

from matplotlib.patches import Circle

F=plt.gcf()
axes=F.gca()
F.get_dpi()
defaultSize=F.get_size_inches()
F.set_size_inches(defaultSize*1.5)

# delete previous patches:

axes.patches = []

# rebuild circular markers
largehollowcircles = []
```

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```
smallredcircles = []
# correction only to fit peak position to the display
offset_convention = np.array([1, 1])

XYlist = peaklist[:, :2] - offset_convention

for po in XYlist:

    large_circle = Circle(po, 7, fill=False, color='b')
    center_circle = Circle(po, .5 , fill=True, color='r')
    axes.add_patch(large_circle)
    axes.add_patch(center_circle)

    largehollowcircles.append(large_circle)
    smallredcircles.append(center_circle)
```

```
<IPython.core.display.Javascript object>
```

List of peaks props is written in a file with extension .dat, here the variable is ‘‘datfilename‘‘

```
if imageindex is not None:
    peaklistprefix=prefixfilename+'cor_%04d'%imageindex
else:
    peaklistprefix=imagefilename.split('.')[0]+'Notebook'
print('peaklist.shape',peaklist.shape)
print("fullpathimagefile",fullpathimagefile)
print('imagefolder',imagefolder)
RMCCD.writepeaklist(peaklist,peaklistprefix,outputfolder=imagefolder,
↪initialfilename=fullpathimagefile)

datfilename = peaklistprefix+'.dat'
```

```
peaklist.shape (82, 10)
fullpathimagefile ../LaueImages/Ge_blanc_0000.mccd
imagefolder ../LaueImages
table of 82 peak(s) with 10 columns has been written in
/home/micha/LaueToolsPy3/LaueTools/LaueImages/Ge_blanc_0000Notebook.dat
```

Now indexing

geometry calibration parameters

Either you fill manually the dict of parameters or you read a file .det

```
# detector geometry and parameters as read from Geblanc0000.det
calibration_parameters = [70.775, 941.74, 1082.57, 0.631, -0.681]
CCDCalibdict = {}
CCDCalibdict['CCDCalibParameters'] = calibration_parameters
CCDCalibdict['framedim'] = (2048, 2048)
CCDCalibdict['detectordiameter'] = 165.
CCDCalibdict['kf_direction'] = 'Z>0'
CCDCalibdict['xpixelsize'] = 0.07914

# CCDCalibdict can also be simply build by reading the proper .det file
```

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```
print("reading geometry calibration file")
CCDCalibdict=IOLT.readCalib_det_file(os.path.join(imagefolder,'Geblanc0000.det'))
CCDCalibdict['kf_direction'] = 'Z>0'
```

```
reading geometry calibration file
calib =  [ 7.07760e+01  9.41760e+02  1.08244e+03  6.29000e-01 -6.85000e-01
  7.91400e-02  2.04800e+03  2.04800e+03]
matrix =  [ 0.995829 -0.071471 -0.056709  0.012247  0.720654 -0.693187  0.09041
  0.689602  0.718523]
```

creation of a .cor file containing accurate scattering angles thanks to detector geometry parameters

Only list of spots with scattering angles can be indexed. In LaueTools .dat file contains only X, Y pixel positions, .cor file contains in addition 2theta and chi scattering angles, and .fit file in addition indexed results properties (such as h, k, l, energy, grain index ...)

```
import LaueTools.LaueGeometry as LTGeo
LTGeo.convert2corfile(datfilename,
                        calibration_parameters,
                        dirname_in=imagefolder,
                       dirname_out=imagefolder,
                       CCDCalibdict=CCDCalibdict)
corfilename = datfilename.split('.')[0] + '.cor'
fullpathcorfile = os.path.join(imagefolder,corfilename)
```

```
Entering CrystalParameters **---**********************


nb of spots and columns in .dat file (82, 3)
file :../LaueImages/Ge_blanc_0000Notebook.dat
containing 82 peaks
(2theta chi X Y I) written in ../LaueImages/Ge_blanc_0000Notebook.cor
```

create instance of an objet spotsset class

```
import LaueTools.indexingSpotsSet as ISS
DataSet = ISS.spotsset()

DataSet.importdatafromfile(fullpathcorfile)
```

```
Cython compiled module for fast computation of Laue spots is not installed!
Cython compiled 'angulardist' module for fast computation of angular distance is not␣
↪installed!
Using default module
Cython compiled module for fast computation of angular distance is not installed!
module Image / PIL is not installed
CCDcalib in readfile_cor {'dd': 70.776, 'xcen': 941.76, 'ycen': 1082.44, 'xbet': 0.
↪629, 'xgam': -0.685, 'xpixelsize': 0.07914, 'ypixelsize': 0.07914, 'CCDLabel':
↪'MARCCD165', 'framedim': [2048.0, 2048.0], 'detectordiameter': 162.07872, 'kf_
↪direction': 'Z>0', 'pixelsize': 0.07914}
CCD Detector parameters read from .cor file
CCDcalibdict {'dd': 70.776, 'xcen': 941.76, 'ycen': 1082.44, 'xbet': 0.629, 'xgam': -
↪0.685, 'xpixelsize': 0.07914, 'ypixelsize': 0.07914, 'CCDLabel': 'MARCCD165',
↪'framedim': [2048.0, 2048.0], 'detectordiameter': 162.07872, 'kf_direction': 'Z>0',
↪'pixelsize': 0.07914}
```

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```
True
```

```
DataSet.getUnIndexedSpotsallData()[:3]
```

```
array([[ 0.0000000e+00,  5.8426915e+01,  2.0130035e+01,  6.2313000e+02,
         1.6577300e+03,  2.9799380e+04],
       [ 1.0000000e+00,  5.7634672e+01, -1.8415523e+01,  1.2443300e+03,
         1.6621500e+03,  2.2425630e+04],
       [ 2.0000000e+00,  8.0919846e+01,  6.6158100e-01,  9.3304000e+02,
         1.2154400e+03,  2.2197540e+04]])
```

Set parameters for indexation: Ge, maximum energy

All materials are listed in dict_LaueTools.py in dict_Materials. You can edit/modify the module (then a restart of the kernel is necessary)

```
emin=5
# emax can be lowered for large unit cell indexation (but greater than BM32 highest␣
↪energy is meaningless)
emax=22
# key of materials
key_material='Ge'

dict_indexrefine = {# recognition angle parameters from two sets A and B
                    'AngleTolLUT': 0.5,
                    'nlutmax':3,
                    'central spots indices': [0,1,2,3,4],  # spots set A
                    'NBMAXPROBED': 10,  # spots set B
                    'MATCHINGRATE_ANGLE_TOL': 0.2,
                 # refinement parameters (loop over narrower matching angles)
                    'list matching tol angles':[0.5,0.2,0.1],

                 # minor parameters
                 'MATCHINGRATE_THRESHOLD_IAL': 100,
                    'UseIntensityWeights': False,
                    'nbSpotsToIndex':10000,
                    'MinimumNumberMatches': 3,
                    'MinimumMatchingRate':3
                    }

#
grainindex=0
DataSet = ISS.spotsset()

DataSet.pixelsize = CCDCalibdict['xpixelsize']
DataSet.dim = CCDCalibdict['framedim']
DataSet.detectordiameter = CCDCalibdict['detectordiameter']
DataSet.kf_direction = CCDCalibdict['kf_direction']
DataSet.key_material = key_material
DataSet.emin = emin
DataSet.emax = emax
```

Before launching the indexation procedure you may want to check a solution found elsewhere or sometimes ago. Then fill ‘‘previousResults‘‘ as shown below

```
#CheckFirstThisMatrix=np.array([[-0.44486058225058 ,  0.098996190230096 ,-0.
↪897868909077371],[-0.883970521873963,0.1130536332378 , 0.462465547362675],
# [ 0.143878606007886, 0.993706753289519 , 0.0350648092250 47]])

# nb of matrices, list of matrices to check, dummy parameter, dummy parameter
#previousResults = 1,[CheckFirstThisMatrix],50,50


previousResults = None
```

Then launch indexation by specifying some arguments of the method ‘‘IndexSpotsSet‘‘:

```
- nbGrainstoFind: nb of grains of this material you want to find
- set_central_spots_hkl: imposed miller indices [h,k,l] of central spots (set A of␣
↪spots)  else : None
...
```

```
t0 =time.time()

DataSet.IndexSpotsSet(fullpathcorfile, key_material, emin, emax, dict_indexrefine,␣
↪None,
                          use_file=1, # read .cor file and reset also spots properties␣
↪dictionary
                          IMM=False,LUT=None,n_LUT=dict_indexrefine['nlutmax'],
↪angletol_list=dict_indexrefine['list matching tol angles'],
                        nbGrainstoFind=1,  # nb of grains of the same material in␣
↪this case
                        set_central_spots_hkl=[0,1,1],  # set hkl of spots of set A
                        MatchingRate_List=[10, 10, 10,10,10,10,10,10],  # minimum␣
↪matching rate figure to keep on looping for refinement
                        verbose=0,
                        previousResults=previousResults, # check before the␣
↪orientation if not None
                        corfilename=corfilename)

# write unindexed spots list in a .cor file
DataSet.writecorFile_unindexedSpots(corfilename=corfilename,
                                                dirname=imagefolder,
                                                filename_nbdigits=4)

# write .fit file of indexed spots belonging to grain #0
DataSet.writeFitFile(0,corfilename=corfilename,dirname=imagefolder)

tf = time.time()-t0
```

```
CCDcalib in readfile_cor {'dd': 70.776, 'xcen': 941.76, 'ycen': 1082.44,␣
↪'xbet': 0.629, 'xgam': -0.685, 'xpixelsize': 0.07914, 'ypixelsize': 0.07914,
↪ 'CCDLabel': 'MARCCD165', 'framedim': [2048.0, 2048.0], 'detectordiameter':␣
↪162.07872, 'kf_direction': 'Z>0', 'pixelsize': 0.07914}
CCD Detector parameters read from .cor file
CCDcalibdict {'dd': 70.776, 'xcen': 941.76, 'ycen': 1082.44, 'xbet': 0.629,␣
↪'xgam': -0.685, 'xpixelsize': 0.07914, 'ypixelsize': 0.07914, 'CCDLabel':␣
↪'MARCCD165', 'framedim': [2048.0, 2048.0], 'detectordiameter': 162.07872,␣
↪'kf_direction': 'Z>0', 'pixelsize': 0.07914}
self.pixelsize in IndexSpotsSet 0.07914
ResolutionAngstromLUT in IndexSpotsSet False
```

```
 Remaining nb of spots to index for grain #0 : 82


 **
start to index grain #0 of Material: Ge

**

providing new set of matrices Using Angles LUT template matching
nbspots 82
NBMAXPROBED 10
nbspots 82
set_central_spots_hkl [0, 1, 1]
Central set of exp. spotDistances from spot_index_central_list probed
self.absolute_index [ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18␣
↪19 20 21 22 23
 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47
 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71
 72 73 74 75 76 77 78 79 80 81]
spot_index_central_list [0, 1, 2, 3, 4]
[0 1 2 3 4]
LUT is None when entering getOrientMatrices()
set_central_spots_hkl [0, 1, 1]
set_central_spots_hkl is not None in getOrientMatrices()
set_central_spots_hkl [0 1 1]
set_central_spots_hkl.shape (3,)
case: 1a
set_central_spots_hkl_list [[0 1 1]
 [0 1 1]
 [0 1 1]
 [0 1 1]
 [0 1 1]]
cubicSymmetry True
LUT_tol_angle 0.5
---***--------------------------------------------------*
Calculating all possible matrices from exp spot #0 and the 9 other(s)
hkl in getOrientMatrices [0 1 1] <class 'numpy.ndarray'>
using LUTspecific
LUTspecific is None for k_centspot_index 0 in getOrientMatrices()
hkl1 in matrices_from_onespot_hkl() [0 1 1]
Computing hkl2 list for specific or cubic LUT in matrices_from_onespot_hkl()
Calculating LUT in PlanePairs_from2sets()
Looking up planes pairs in LUT from exp. spots (0, 2):
Looking up planes pairs in LUT from exp. spots (0, 6):
Looking up planes pairs in LUT from exp. spots (0, 9):
calculating matching rates of solutions for exp. spots [0, 2]
calculating matching rates of solutions for exp. spots [0, 6]
calculating matching rates of solutions for exp. spots [0, 9]


---***--------------------------------------------------*
Calculating all possible matrices from exp spot #1 and the 9 other(s)
hkl in getOrientMatrices [0 1 1] <class 'numpy.ndarray'>
using LUTspecific
```

```
LUTspecific is not None for k_centspot_index 1 in getOrientMatrices()
hkl1 in matrices_from_onespot_hkl() [0 1 1]
Using specific LUT in matrices_from_onespot_hkl()
Looking up planes pairs in LUT from exp. spots (1, 2):
Looking up planes pairs in LUT from exp. spots (1, 7):
Looking up planes pairs in LUT from exp. spots (1, 9):
calculating matching rates of solutions for exp. spots [1, 2]
calculating matching rates of solutions for exp. spots [1, 7]
calculating matching rates of solutions for exp. spots [1, 9]


---***-------------------------------------------------*
Calculating all possible matrices from exp spot #2 and the 9 other(s)
hkl in getOrientMatrices [0 1 1] <class 'numpy.ndarray'>
using LUTspecific
LUTspecific is not None for k_centspot_index 2 in getOrientMatrices()
hkl1 in matrices_from_onespot_hkl() [0 1 1]
Using specific LUT in matrices_from_onespot_hkl()
Looking up planes pairs in LUT from exp. spots (2, 0):
Looking up planes pairs in LUT from exp. spots (2, 1):
Looking up planes pairs in LUT from exp. spots (2, 9):
calculating matching rates of solutions for exp. spots [2, 0]
calculating matching rates of solutions for exp. spots [2, 1]
calculating matching rates of solutions for exp. spots [2, 9]


---***-------------------------------------------------*
Calculating all possible matrices from exp spot #3 and the 9 other(s)
hkl in getOrientMatrices [0 1 1] <class 'numpy.ndarray'>
using LUTspecific
LUTspecific is not None for k_centspot_index 3 in getOrientMatrices()
hkl1 in matrices_from_onespot_hkl() [0 1 1]
Using specific LUT in matrices_from_onespot_hkl()
Looking up planes pairs in LUT from exp. spots (3, 7):
Looking up planes pairs in LUT from exp. spots (3, 8):
Looking up planes pairs in LUT from exp. spots (3, 9):
calculating matching rates of solutions for exp. spots [3, 7]
calculating matching rates of solutions for exp. spots [3, 8]
calculating matching rates of solutions for exp. spots [3, 9]


---***-------------------------------------------------*
Calculating all possible matrices from exp spot #4 and the 9 other(s)
hkl in getOrientMatrices [0 1 1] <class 'numpy.ndarray'>
using LUTspecific
LUTspecific is not None for k_centspot_index 4 in getOrientMatrices()
hkl1 in matrices_from_onespot_hkl() [0 1 1]
Using specific LUT in matrices_from_onespot_hkl()
Looking up planes pairs in LUT from exp. spots (4, 6):
Looking up planes pairs in LUT from exp. spots (4, 8):
Looking up planes pairs in LUT from exp. spots (4, 9):
calculating matching rates of solutions for exp. spots [4, 6]
calculating matching rates of solutions for exp. spots [4, 8]
calculating matching rates of solutions for exp. spots [4, 9]
```

```
----------------------------------------
results:
matrix:                                                 matching results
[ 0.071442298339536 -0.056791122889477 -0.995826674863109]        res: [94.0,␣
↪135.0] 0.005 69.63
[-0.720597705663885 -0.693247631822884 -0.012110638459969]        spot␣
↪indices [0 9]
[-0.689608632382347  0.718518569419943 -0.090393581312322]        planes [[-2.
↪0, 1.0, 1.0], [0.0, 1.0, 1.0]]

[ 0.071284911945937 -0.056791915954001 -0.995837908301915]        res: [93.0,␣
↪134.0] 0.006 69.40
[-0.720581964957976 -0.693265307713712 -0.012035152592104]        spot␣
↪indices [1 9]
[-0.68968586701208   0.718453369664079 -0.09032253573791 ]        planes [[-1.
↪0, 2.0, 1.0], [0.0, 1.0, 1.0]]

[-0.071331310042019 -0.995834915200135 -0.056786141584281]        res: [93.0,␣
↪134.0] 0.005 69.40
[ 0.720561755804718 -0.012058289359476 -0.693285910522741]        spot␣
↪indices [2 9]
[ 0.689652960030445 -0.090345399841628  0.718482082900264]        planes [[1.
↪0, 1.0, 1.0], [0.0, 1.0, 1.0]]

[-0.071391558888759 -0.995830258190095 -0.056792096214888]        res: [94.0,␣
↪135.0] 0.006 69.63
[ 0.720671448854468 -0.012140732995851 -0.693170444701969]        spot␣
↪indices [3 9]
[ 0.689588625514858 -0.090412962995124  0.718535332243983]        planes [[2.
↪0, 3.0, 1.0], [0.0, 1.0, 1.0]]

[ 0.071340651481789 -0.056823338834159 -0.995832124210648]        res: [94.0,␣
↪135.0] 0.005 69.63
[-0.720605825766681 -0.693235936569283 -0.012295532523216]        spot␣
↪indices [4 9]
[-0.689563524109094  0.718557247109645 -0.090430242974657]        planes [[-1.
↪0, 2.0, 3.0], [0.0, 1.0, 1.0]]

Number of matrices found (nb_sol):  5
set_central_spots_hkl in FindOrientMatrices [0, 1, 1]
Merging matrices
keep_only_equivalent = False
sorting according to rank
rank [0 4 3 2 1]

----------------------------------------
results:
matrix:                                                 matching results
[ 0.071442298339536 -0.056791122889477 -0.995826674863109]        res: [ 94.␣
↪135.] 0.005 69.63
[-0.720597705663885 -0.693247631822884 -0.012110638459969]
```

```
[-0.689608632382347  0.718518569419943 -0.090393581312322]

[ 0.071340651481789 -0.056823338834159 -0.995832124210648]        res: [ 94.␣
↪135.] 0.005 69.63
[-0.720605825766681 -0.693235936569283 -0.012295532523216]
[-0.689563524109094  0.718557247109645 -0.090430242974657]

[-0.071391558888759 -0.995830258190095 -0.056792096214888]        res: [ 94.␣
↪135.] 0.006 69.63
[ 0.720671448854468 -0.012140732995851 -0.693170444701969]
[ 0.689588625514858 -0.090412962995124  0.718535332243983]

[-0.071331310042019 -0.995834915200135 -0.056786141584281]        res: [ 93.␣
↪134.] 0.005 69.40
[ 0.720561755804718 -0.012058289359476 -0.693285910522741]
[ 0.689652960030445 -0.090345399841628  0.718482082900264]

[ 0.071284911945937 -0.056791915954001 -0.995837908301915]        res: [ 93.␣
↪134.] 0.006 69.40
[-0.720581964957976 -0.693265307713712 -0.012035152592104]
[-0.68968586701208   0.718453369664079 -0.09032253573791 ]

Nb of potential orientation matrice(s) UB found: 5
[[[ 0.071442298339536 -0.056791122889477 -0.995826674863109]
  [-0.720597705663885 -0.693247631822884 -0.012110638459969]
  [-0.689608632382347  0.718518569419943 -0.090393581312322]]

 [[ 0.071340651481789 -0.056823338834159 -0.995832124210648]
  [-0.720605825766681 -0.693235936569283 -0.012295532523216]
  [-0.689563524109094  0.718557247109645 -0.090430242974657]]

 [[-0.071391558888759 -0.995830258190095 -0.056792096214888]
  [ 0.720671448854468 -0.012140732995851 -0.693170444701969]
  [ 0.689588625514858 -0.090412962995124  0.718535332243983]]

 [[-0.071331310042019 -0.995834915200135 -0.056786141584281]
  [ 0.720561755804718 -0.012058289359476 -0.693285910522741]
  [ 0.689652960030445 -0.090345399841628  0.718482082900264]]

 [[ 0.071284911945937 -0.056791915954001 -0.995837908301915]
  [-0.720581964957976 -0.693265307713712 -0.012035152592104]
  [-0.68968586701208   0.718453369664079 -0.09032253573791 ]]]
Nb of potential UBs  5

Working with a new stack of orientation matrices
MATCHINGRATE_THRESHOLD_IAL= 100.0
has not been reached! All potential solutions have been calculated
taking the first one only.
bestUB object <LaueTools.indexingSpotsSet.OrientMatrix object at␣
↪0x7f7c954f5e80>


---------------refining grain orientation and strain #0-----------------
```

```
 refining grain #0 step -----0

bestUB <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7f7c954f5e80>
True it is an OrientMatrix object
Orientation <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7f7c954f5e80>
matrix [[-0.071391558888759 -0.995830258190095 -0.056792096214888]
 [ 0.720671448854468 -0.012140732995851 -0.693170444701969]
 [ 0.689588625514858 -0.090412962995124  0.718535332243983]]
***nb of selected spots in AssignHKL*** 82
UBOrientMatrix [[-0.071391558888759 -0.995830258190095 -0.056792096214888]
 [ 0.720671448854468 -0.012140732995851 -0.693170444701969]
 [ 0.689588625514858 -0.090412962995124  0.718535332243983]]
For angular tolerance 0.50 deg
Nb of pairs found / nb total of expected spots: 81/147
Matching Rate : 55.10
Nb missing reflections: 66

grain #0 : 81 links to simulated spots have been found
*********mean pixel deviation    0.2522039400422887     ******
Initial residues [0.191356096913678 0.158479888122211 0.125984922997516 0.
↪007464331088751
 0.220920883122328 0.065197410024489 0.405464259132319 0.079769518806149
 0.309835172580193 0.024815180122634 0.146635771529913 0.197926454567734
 0.253815574123594 0.241517985294699 0.301875442673439 0.217498144625921
 0.186026257638361 0.152430964466482 0.022468745875909 0.372498387808433
 0.225884815274198 0.155682523936061 0.308213213363587 0.354423361607117
 0.237793437184287 0.344146246502948 0.117700835663451 0.22732103372742
 0.263538267437741 0.133994037769124 0.091015982918167 0.367309714380722
 0.359174426753832 0.281533512444384 0.191021625928391 0.219461033259323
 0.371983339466526 0.3512796731268   0.298580209240117 0.447936020775024
 0.160438308161376 0.631208433750478 0.420060120050684 0.195238104695171
 0.051118832992816 0.159003375870547 0.354123955360538 0.049380652521924
 0.301744705672337 0.127112320459672 0.082920786835417 0.19281838475986
 0.130182524243209 0.332360152782496 0.533160923855596 0.276782907418236
 0.125265672564509 0.184320173657227 0.238789408490181 0.149666955002009
 0.473603697641706 0.235878500572685 0.425250385266374 0.445829965130009
 0.255853120078437 0.271987274130697 0.298711159306184 0.310382741777609
 0.228936459666657 0.374245425300233 0.100039587285176 0.096572087547537
 0.196098380129156 0.140612883827292 0.338936919946618 0.526244208385607
 0.190627233723994 0.629487817359844 0.233333060530866 0.316852495355672
 0.61336433904477 ]
--------------------------------------------------



**********************
first error with initial values of: ['b/a', 'c/a', 'a12', 'a13', 'a23',␣
↪'theta1', 'theta2', 'theta3']

**********************

*********mean pixel deviation    0.2522039400422887     ******
```

```
**********************
Fitting parameters:   ['b/a', 'c/a', 'a12', 'a13', 'a23', 'theta1', 'theta2',␣
↪'theta3']

**********************

With initial values [1. 1. 0. 0. 0. 0. 0. 0.]
code results 1
nb iterations 189
mesg Both actual and predicted relative reductions in the sum of squares
  are at most 0.000000
strain_sol [ 9.999862096544356e-01  9.999941276097474e-01 -7.144700897145182e-
↪06
  5.728542645493929e-05  1.242229382006964e-05  2.977984275077042e-05
 -1.953472667313407e-03  6.919002586889341e-03]


 **********  End of Fitting  -  Final errors  **************


**********mean pixel deviation    0.18215488925149526     ******
devstrain, lattice_parameter_direct_strain [[-4.815998025634964e-06  5.
↪250997004746657e-06 -2.870284279887629e-05]
 [ 5.250997004746657e-06  7.352907498721824e-06 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06 -2.536909473086861e-06]] [ 5.
↪657509728355469  5.657578574250457  5.657522951317707
 90.0010541881893   90.00328909016345  89.99939828842365 ]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.6575            5.657568845776604  5.
↪6575132229395
 90.0010541881893   90.00328909016345  89.99939828842365 ]
devstrain1, lattice_parameter_direct_strain1 [[-4.815998025634964e-06  5.
↪250997004746657e-06 -2.870284279887629e-05]
 [ 5.250997004746657e-06  7.352907498721824e-06 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06 -2.536909473086861e-06]] [ 5.
↪6575             5.657568845776604  5.6575132229395
 90.0010541881893   90.00328909016345  89.99939828842365 ]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[ 1.719550237533340e-06  5.250997004746657e-06 -2.
↪870284279887629e-05]
 [ 5.250997004746657e-06  1.388845576189013e-05 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06  3.998638790081444e-06]]
deviatoric strain [[-4.815998025634964e-06  5.250997004746657e-06 -2.
↪870284279887629e-05]
 [ 5.250997004746657e-06  7.352907498721824e-06 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06 -2.536909473086861e-06]]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[ 1.719550237533340e-06  5.250997004746657e-06 -2.
↪870284279887629e-05]
 [ 5.250997004746657e-06  1.388845576189013e-05 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06  3.998638790081444e-06]]
deviatoric strain [[-4.815998025634964e-06  5.250997004746657e-06 -2.
```

```
 ↪870284279887629e-05]
  [ 5.250997004746657e-06  7.352907498721824e-06 -9.199263307200638e-06]
  [-2.870284279887629e-05 -9.199263307200638e-06 -2.536909473086861e-06]]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
 ↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.6575             5.657568845776604  5.
 ↪6575132229395
  90.0010541881893   90.00328909016345  89.99939828842365 ]
final lattice_parameters [ 5.6575             5.657568845776604  5.
 ↪6575132229395
  90.0010541881893   90.00328909016345  89.99939828842365 ]
UB and strain refinement completed
True it is an OrientMatrix object
Orientation <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7f7c851edeb8>
matrix [[-0.071478224945242 -0.995814588672313 -0.056724144676328]
  [ 0.720639310822985 -0.012262885888099 -0.693156594892675]
  [ 0.689613233174427 -0.090416539541802  0.718545890295648]]
*nb of selected spots in AssignHKL*** 82
UBOrientMatrix [[-0.071478224945242 -0.995814588672313 -0.056724144676328]
  [ 0.720639310822985 -0.012262885888099 -0.693156594892675]
  [ 0.689613233174427 -0.090416539541802  0.718545890295648]]
For angular tolerance 0.50 deg
Nb of pairs found / nb total of expected spots: 81/147
Matching Rate : 55.10
Nb missing reflections: 66

grain #0 : 81 links to simulated spots have been found
GoodRefinement condition is  True
nb_updates 81 compared to 6


 refining grain #0 step -----1

bestUB <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7f7c954f5e80>
True it is an OrientMatrix object
Orientation <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7f7c954f5e80>
matrix [[-0.071391558888759 -0.995830258190095 -0.056792096214888]
  [ 0.720671448854468 -0.012140732995851 -0.693170444701969]
  [ 0.689588625514858 -0.090412962995124  0.718535332243983]]
*nb of selected spots in AssignHKL*** 82
UBOrientMatrix [[-0.071391558888759 -0.995830258190095 -0.056792096214888]
  [ 0.720671448854468 -0.012140732995851 -0.693170444701969]
  [ 0.689588625514858 -0.090412962995124  0.718535332243983]]
For angular tolerance 0.20 deg
Nb of pairs found / nb total of expected spots: 81/147
Matching Rate : 55.10
Nb missing reflections: 66

grain #0 : 81 links to simulated spots have been found
*********mean pixel deviation    0.2522039400422887     ******
Initial residues [0.191356096913678 0.158479888122211 0.125984922997516 0.
 ↪007464331088751
  0.220920883122328 0.065197410024489 0.405464259132319 0.079769518806149
  0.309835172580193 0.024815180122634 0.146635771529913 0.197926454567734
```

```
 0.253815574123594 0.241517985294699 0.301875442673439 0.217498144625921
 0.186026257638361 0.152430964466482 0.022468745875909 0.372498387808433
 0.225884815274198 0.155682523936061 0.308213213363587 0.354423361607117
 0.237793437184287 0.344146246502948 0.117700835663451 0.22732103372742
 0.263538267437741 0.133994037769124 0.091015982918167 0.367309714380722
 0.359174426753832 0.281533512444384 0.191021625928391 0.219461033259323
 0.371983339466526 0.3512796731268   0.298580209240117 0.447936020775024
 0.160438308161376 0.631208433750478 0.420060120050684 0.195238104695171
 0.051118832992816 0.159003375870547 0.354123955360538 0.049380652521924
 0.301744705672337 0.127112320459672 0.082920786835417 0.19281838475986
 0.130182524243209 0.332360152782496 0.533160923855596 0.276782907418236
 0.125265672564509 0.184320173657227 0.238789408490181 0.149666955002009
 0.473603697641706 0.235878500572685 0.425250385266374 0.445829965130009
 0.255853120078437 0.271987274130697 0.298711159306184 0.310382741777609
 0.228936459666657 0.374245425300233 0.100039587285176 0.096572087547537
 0.196098380129156 0.140612883827292 0.338936919946618 0.526244208385607
 0.190627233723994 0.629487817359844 0.233333060530866 0.316852495355672
 0.61336433904477 ]
--------------------------------------------------
```

```
**********
first error with initial values of: ['b/a', 'c/a', 'a12', 'a13', 'a23',␣
↪'theta1', 'theta2', 'theta3']

**********

*********mean pixel deviation    0.2522039400422887     ******


**********
Fitting parameters:   ['b/a', 'c/a', 'a12', 'a13', 'a23', 'theta1', 'theta2',␣
↪'theta3']

**********

With initial values [1. 1. 0. 0. 0. 0. 0. 0.]
code results 1
nb iterations 189
mesg Both actual and predicted relative reductions in the sum of squares
  are at most 0.000000
strain_sol [ 9.999862096544356e-01  9.999941276097474e-01 -7.144700897145182e-
↪06
  5.728542645493929e-05  1.242229382006964e-05  2.977984275077042e-05
 -1.953472667313407e-03  6.919002586889341e-03]


 **********  End of Fitting  -  Final errors  **************


*********mean pixel deviation    0.18215488925149526     ******
devstrain, lattice_parameter_direct_strain [[-4.815998025634964e-06  5.
↪250997004746657e-06 -2.870284279887629e-05]
```

```
 [ 5.250997004746657e-06  7.352907498721824e-06 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06 -2.536909473086861e-06]] [ 5.
↪657509728355469  5.657578574250457  5.657522951317707
 90.0010541881893   90.00328909016345  89.99939828842365 ]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.6575            5.657568845776604  5.
↪6575132229395
 90.0010541881893   90.00328909016345  89.99939828842365 ]
devstrain1, lattice_parameter_direct_strain1 [[-4.815998025634964e-06  5.
↪250997004746657e-06 -2.870284279887629e-05]
 [ 5.250997004746657e-06  7.352907498721824e-06 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06 -2.536909473086861e-06]] [ 5.
↪6575             5.657568845776604  5.6575132229395
 90.0010541881893   90.00328909016345  89.99939828842365 ]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[ 1.719550237533340e-06  5.250997004746657e-06 -2.
↪870284279887629e-05]
 [ 5.250997004746657e-06  1.388845576189013e-05 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06  3.998638790081444e-06]]
deviatoric strain [[-4.815998025634964e-06  5.250997004746657e-06 -2.
↪870284279887629e-05]
 [ 5.250997004746657e-06  7.352907498721824e-06 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06 -2.536909473086861e-06]]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[ 1.719550237533340e-06  5.250997004746657e-06 -2.
↪870284279887629e-05]
 [ 5.250997004746657e-06  1.388845576189013e-05 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06  3.998638790081444e-06]]
deviatoric strain [[-4.815998025634964e-06  5.250997004746657e-06 -2.
↪870284279887629e-05]
 [ 5.250997004746657e-06  7.352907498721824e-06 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06 -2.536909473086861e-06]]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.6575            5.657568845776604  5.
↪6575132229395
 90.0010541881893   90.00328909016345  89.99939828842365 ]
final lattice_parameters [ 5.6575            5.657568845776604  5.
↪6575132229395
 90.0010541881893   90.00328909016345  89.99939828842365 ]
UB and strain refinement completed
True it is an OrientMatrix object
Orientation <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7f7c84338898>
matrix [[-0.071478224945242 -0.995814588672313 -0.056724144676328]
 [ 0.720639310822985 -0.012262885888099 -0.693156594892675]
 [ 0.689613233174427 -0.090416539541802  0.718545890295648]]
***nb of selected spots in AssignHKL*** 82
UBOrientMatrix [[-0.071478224945242 -0.995814588672313 -0.056724144676328]
 [ 0.720639310822985 -0.012262885888099 -0.693156594892675]
 [ 0.689613233174427 -0.090416539541802  0.718545890295648]]
For angular tolerance 0.20 deg
Nb of pairs found / nb total of expected spots: 81/147
Matching Rate : 55.10
```

```
Nb missing reflections: 66

grain #0 : 81 links to simulated spots have been found
GoodRefinement condition is  True
nb_updates 81 compared to 6


 refining grain #0 step -----2

bestUB <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7f7c954f5e80>
True it is an OrientMatrix object
Orientation <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7f7c954f5e80>
matrix [[-0.071391558888759 -0.995830258190095 -0.056792096214888]
 [ 0.720671448854468 -0.012140732995851 -0.693170444701969]
 [ 0.689588625514858 -0.090412962995124  0.718535332243983]]
*nb of selected spots in AssignHKL*** 82
UBOrientMatrix [[-0.071391558888759 -0.995830258190095 -0.056792096214888]
 [ 0.720671448854468 -0.012140732995851 -0.693170444701969]
 [ 0.689588625514858 -0.090412962995124  0.718535332243983]]
For angular tolerance 0.10 deg
Nb of pairs found / nb total of expected spots: 81/147
Matching Rate : 55.10
Nb missing reflections: 66

grain #0 : 81 links to simulated spots have been found
*********mean pixel deviation    0.2522039400422887     ******
Initial residues [0.191356096913678 0.158479888122211 0.125984922997516 0.
↪007464331088751
 0.220920883122328 0.065197410024489 0.405464259132319 0.079769518806149
 0.309835172580193 0.024815180122634 0.146635771529913 0.197926454567734
 0.253815574123594 0.241517985294699 0.301875442673439 0.217498144625921
 0.186026257638361 0.152430964466482 0.022468745875909 0.372498387808433
 0.225884815274198 0.155682523936061 0.308213213363587 0.354423361607117
 0.237793437184287 0.344146246502948 0.117700835663451 0.22732103372742
 0.263538267437741 0.133994037769124 0.091015982918167 0.367309714380722
 0.359174426753832 0.281533512444384 0.191021625928391 0.219461033259323
 0.371983339466526 0.3512796731268   0.298580209240117 0.447936020775024
 0.160438308161376 0.631208433750478 0.420060120050684 0.195238104695171
 0.051118832992816 0.159003375870547 0.354123955360538 0.049380652521924
 0.301744705672337 0.127112320459672 0.082920786835417 0.19281838475986
 0.130182524243209 0.332360152782496 0.533160923855596 0.276782907418236
 0.125265672564509 0.184320173657227 0.238789408490181 0.149666955002009
 0.473603697641706 0.235878500572685 0.425250385266374 0.445829965130009
 0.255853120078437 0.271987274130697 0.298711159306184 0.310382741777609
 0.228936459666657 0.374245425300233 0.100039587285176 0.096572087547537
 0.196098380129156 0.140612883827292 0.338936919946618 0.526244208385607
 0.190627233723994 0.629487817359844 0.233333060530866 0.316852495355672
 0.61336433904477 ]
----------------------------------------------------


**********************
first error with initial values of: ['b/a', 'c/a', 'a12', 'a13', 'a23',␣
```

```
 ↪'theta1', 'theta2', 'theta3']

**********************

*********mean pixel deviation    0.2522039400422887     ******


**********************
Fitting parameters:   ['b/a', 'c/a', 'a12', 'a13', 'a23', 'theta1', 'theta2',␣
 ↪'theta3']

**********************

With initial values [1. 1. 0. 0. 0. 0. 0. 0.]
code results 1
nb iterations 189
mesg Both actual and predicted relative reductions in the sum of squares
  are at most 0.000000
strain_sol [ 9.999862096544356e-01  9.999941276097474e-01 -7.144700897145182e-
 ↪06
  5.728542645493929e-05  1.242229382006964e-05  2.977984275077042e-05
 -1.953472667313407e-03  6.919002586889341e-03]


 **********  End of Fitting  -  Final errors  **************


*********mean pixel deviation    0.18215488925149526     ******
devstrain, lattice_parameter_direct_strain [[-4.815998025634964e-06  5.
 ↪250997004746657e-06 -2.870284279887629e-05]
 [ 5.250997004746657e-06  7.352907498721824e-06 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06 -2.536909473086861e-06]] [ 5.
 ↪657509728355469  5.657578574250457  5.657522951317707
 90.0010541881893   90.00328909016345  89.99939828842365 ]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
 ↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.6575            5.657568845776604  5.
 ↪6575132229395
 90.0010541881893   90.00328909016345  89.99939828842365 ]
devstrain1, lattice_parameter_direct_strain1 [[-4.815998025634964e-06  5.
 ↪250997004746657e-06 -2.870284279887629e-05]
 [ 5.250997004746657e-06  7.352907498721824e-06 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06 -2.536909473086861e-06]] [ 5.
 ↪6575             5.657568845776604  5.6575132229395
 90.0010541881893   90.00328909016345  89.99939828842365 ]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[ 1.719550237533340e-06  5.250997004746657e-06 -2.
 ↪870284279887629e-05]
 [ 5.250997004746657e-06  1.388845576189013e-05 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06  3.998638790081444e-06]]
deviatoric strain [[-4.815998025634964e-06  5.250997004746657e-06 -2.
 ↪870284279887629e-05]
 [ 5.250997004746657e-06  7.352907498721824e-06 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06 -2.536909473086861e-06]]
```

```
new UBs matrix in q= UBs G (s for strain)
strain_direct [[ 1.719550237533340e-06  5.250997004746657e-06 -2.
↪870284279887629e-05]
 [ 5.250997004746657e-06  1.388845576189013e-05 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06  3.998638790081444e-06]]
deviatoric strain [[-4.815998025634964e-06  5.250997004746657e-06 -2.
↪870284279887629e-05]
 [ 5.250997004746657e-06  7.352907498721824e-06 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06 -2.536909473086861e-06]]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.6575            5.657568845776604  5.
↪6575132229395
 90.0010541881893   90.00328909016345  89.99939828842365 ]
final lattice_parameters [ 5.6575            5.657568845776604  5.
↪6575132229395
 90.0010541881893   90.00328909016345  89.99939828842365 ]
UB and strain refinement completed
True it is an OrientMatrix object
Orientation <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7f7c94485da0>
matrix [[-0.071478224945242 -0.995814588672313 -0.056724144676328]
 [ 0.720639310822985 -0.012262885888099 -0.693156594892675]
 [ 0.689613233174427 -0.090416539541802  0.718545890295648]]
***nb of selected spots in AssignHKL*** 81
UBOrientMatrix [[-0.071478224945242 -0.995814588672313 -0.056724144676328]
 [ 0.720639310822985 -0.012262885888099 -0.693156594892675]
 [ 0.689613233174427 -0.090416539541802  0.718545890295648]]
For angular tolerance 0.10 deg
Nb of pairs found / nb total of expected spots: 81/147
Matching Rate : 55.10
Nb missing reflections: 66

grain #0 : 81 links to simulated spots have been found
GoodRefinement condition is  True
nb_updates 81 compared to 6

-------------------------------------------
indexing completed for grain #0 with matching rate 55.10
-------------------------------------------

writing fit file -------------------------
for grainindex= 0
self.dict_grain_matrix[grain_index] [[-0.071478224945242 -0.995814588672313 -
↪0.056724144676328]
 [ 0.720639310822985 -0.012262885888099 -0.693156594892675]
 [ 0.689613233174427 -0.090416539541802  0.718545890295648]]
self.refinedUBmatrix [[-0.071478224945242 -0.995814588672313 -0.
↪056724144676328]
 [ 0.720639310822985 -0.012262885888099 -0.693156594892675]
 [ 0.689613233174427 -0.090416539541802  0.718545890295648]]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[ 1.719550237533340e-06  5.250997004746657e-06 -2.
↪870284279887629e-05]
 [ 5.250997004746657e-06  1.388845576189013e-05 -9.199263307200638e-06]
```

```
 [-2.870284279887629e-05 -9.199263307200638e-06  3.998638790081444e-06]]
deviatoric strain [[-4.815998025634964e-06  5.250997004746657e-06 -2.
↪870284279887629e-05]
 [ 5.250997004746657e-06  7.352907498721824e-06 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06 -2.536909473086861e-06]]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[ 1.719550237533340e-06  5.250997004746657e-06 -2.
↪870284279887629e-05]
 [ 5.250997004746657e-06  1.388845576189013e-05 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06  3.998638790081444e-06]]
deviatoric strain [[-4.815998025634964e-06  5.250997004746657e-06 -2.
↪870284279887629e-05]
 [ 5.250997004746657e-06  7.352907498721824e-06 -9.199263307200638e-06]
 [-2.870284279887629e-05 -9.199263307200638e-06 -2.536909473086861e-06]]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.6575            5.657568845776604  5.
↪6575132229395
 90.0010541881893   90.00328909016345  89.99939828842365 ]
final lattice_parameters [ 5.6575            5.657568845776604  5.
↪6575132229395
 90.0010541881893   90.00328909016345  89.99939828842365 ]
File : Ge_blanc_0000Notebook_g0.fit written in /home/micha/LaueToolsPy3/
↪LaueTools/notebooks
Experimental experimental spots indices which are not indexed []
Missing reflections grainindex is -100 for indexed grainindex 0
within angular tolerance 0.500

 Remaining nb of spots to index for grain #1 : 1

81 spots have been indexed over 82
indexing rate is --- : 98.8 percents
indexation of ../LaueImages/Ge_blanc_0000Notebook.cor is completed
for the 1 grain(s) that has(ve) been indexed as requested
Leaving Index and Refine procedures...
Saving unindexed  fit file: ../LaueImages/Ge_blanc_0000Notebook_unindexed.cor
File : ../LaueImages/Ge_blanc_0000Notebook_g0.fit written in /home/micha/
↪LaueToolsPy3/LaueTools/notebooks
```

```
print('Indexation time %.3f second(s) \n\n'%tf)
print('Spots properties of the 10 first spots that have been indexed (sorted by␣
↪intensity)')
print('#spot 2theta chi X, Y intensity h k l energy')
print(DataSet.getSpotsFamilyallData(0)[:10])
```

```
Indexation time 2.487 second(s)


Spots properties of the 10 first spots that have been indexed (sorted by intensity)
#spot 2theta chi X, Y intensity h k l energy
[[ 0.000000000000000e+00  5.842691500000000e+01  2.013003500000000e+01
   6.231300000000000e+02  1.657730000000000e+03  2.979938000000000e+04
   4.000000000000000e+00  2.000000000000000e+00  2.000000000000000e+00
   1.099874517758171e+01]
```

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```
 [ 1.000000000000000e+00  5.763467200000000e+01 -1.841552300000000e+01
   1.244330000000000e+03  1.662150000000000e+03  2.242563000000000e+04
   2.000000000000000e+00  2.000000000000000e+00  4.000000000000000e+00
   1.113626245226060e+01]
 [ 2.000000000000000e+00  8.091984600000001e+01  6.615810000000000e-01
   9.330400000000000e+02  1.215440000000000e+03  2.219754000000000e+04
   3.000000000000000e+00  3.000000000000000e+00  3.000000000000000e+00
   8.773642495456929e+00]
 [ 3.000000000000000e+00  1.168117220000000e+02  2.128975200000000e+01
   5.852300000000000e+02  5.888000000000000e+02  9.528830000000000e+03
   4.000000000000000e+00  6.000000000000000e+00  2.000000000000000e+00
   9.626187155122841e+00]
 [ 4.000000000000000e+00  1.159585970000000e+02 -2.073868400000000e+01
   1.276610000000000e+03  6.003000000000000e+02  9.153969999999999e+03
   2.000000000000000e+00  6.000000000000000e+00  4.000000000000000e+00
   9.671066779127555e+00]
 [ 5.000000000000000e+00  1.097624120000000e+02  3.270820000000000e-01
   9.326600000000000e+02  7.500800000000000e+02  6.940080000000000e+03
   3.000000000000000e+00  5.000000000000000e+00  3.000000000000000e+00
   8.784305505382406e+00]
 [ 6.000000000000000e+00  9.664626300000000e+01 -3.623969200000000e+01
   1.596620000000000e+03  9.353600000000000e+02  6.136730000000000e+03
   1.000000000000000e+00  5.000000000000000e+00  5.000000000000000e+00
   1.047621498150968e+01]
 [ 7.000000000000000e+00  9.807526100000000e+01  3.749168800000000e+01
   2.523600000000000e+02  9.206000000000000e+02  5.635550000000000e+03
   5.000000000000000e+00  5.000000000000000e+00  1.000000000000000e+00
   1.036136430057910e+01]
 [ 8.000000000000000e+00  6.421410100000000e+01 -1.397936600000000e+01
   1.168360000000000e+03  1.512820000000000e+03  5.570320000000000e+03
   3.000000000000000e+00  3.000000000000000e+00  5.000000000000000e+00
   1.351813316448898e+01]
 [ 9.000000000000000e+00  9.620103100000000e+01 -4.831242900000000e+01
   1.945880000000000e+03  9.142200000000000e+02  5.317320000000000e+03
   0.000000000000000e+00  4.000000000000000e+00  4.000000000000000e+00
   8.328162135695869e+00]]
```

DataSet is an object with many attributes and methods related to spots properties (indexed or not, belonging to grains counted from zero). By press Tab key after having typed DataSet. can show you infos about spots

```
DataSet.B0matrix
```

```
array([[ 1.767565178965975e-01, -2.842461599074922e-17,
        -2.842461599074922e-17],
       [ 0.000000000000000e+00,  1.767565178965975e-01,
        -1.082321519352500e-17],
       [ 0.000000000000000e+00,  0.000000000000000e+00,
         1.767565178965975e-01]])
```

6.2 Indexation of spots data set.

Using Class spotsSet and play with spots considered for indexation and refinement

6.2.1 This Notebook is a part of Tutorials on LaueTools Suite. Author:J.-S. Micha Date: July 2019

```
%matplotlib inline

import matplotlib
import numpy as np
import matplotlib.pyplot as plt
import time,copy,os

# third party LaueTools import
import LaueTools.readmccd as RMCCD
import LaueTools.LaueGeometry as F2TC
import LaueTools.indexingSpotsSet as ISS
import LaueTools.IOLaueTools as RWASCII
```

```
/home/micha/anaconda3/lib/python3.6/site-packages/h5py/__init__.py:36:␣
↪FutureWarning: Conversion of the second argument of issubdtype from float␣
↪to np.floating is deprecated. In future, it will be treated as np.float64␣
↪== np.dtype(float).type.
  from ._conv import register_converters as _register_converters

module Image / PIL is not installed
LaueToolsProjectFolder /home/micha/LaueToolsPy3/LaueTools
Cython compiled module 'gaussian2D' for fast computation is not installed!
module Image / PIL is not installed
Entering CrystalParameters **---**********************


Cython compiled module for fast computation of Laue spots is not installed!
Cython compiled 'angulardist' module for fast computation of angular distance␣
↪is not installed!
Using default module
Cython compiled module for fast computation of angular distance is not␣
↪installed!
module Image / PIL is not installed
```

refinement from guessed solutions with two materials (see script IndexingTwinsSeries)

Let's take a simple example of a single Laue Pattern. From the peak search we get 83 spots

```
folder= '../Examples/Ge/'
datfilename='Ge0001.dat'
```

```
key_material='Ge'
emin, emax= 5,23
```

```
# detector geometry and parameters as read from Ge0001.det
calibration_parameters = [69.179, 1050.81, 1115.59, 0.104, -0.273]
CCDCalibdict = {}
CCDCalibdict['CCDCalibParameters'] = calibration_parameters
CCDCalibdict['framedim'] = (2048, 2048)
CCDCalibdict['detectordiameter'] = 165.
CCDCalibdict['kf_direction'] = 'Z>0'
```

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```
CCDCalibdict['xpixelsize'] = 0.08057
# CCDCalibdict can also be simply build by reading the proper .det file
print("reading geometry calibration file")
CCDCalibdict=RWASCII.readCalib_det_file(os.path.join(folder,'Ge0001.det'))
CCDCalibdict['kf_direction'] = 'Z>0'
```

```
reading geometry calibration file
calib =  [ 6.91790e+01  1.05081e+03  1.11559e+03  1.04000e-01 -2.73000e-01
  8.05700e-02  2.04800e+03  2.04800e+03]
matrix =  [-0.211596  0.092178 -0.973001 -0.77574   0.589743  0.224568  0.594521
  0.802313 -0.053281]
```

Compute scattering angles from spots pixel positions and detector geometry. Write a .cor file from .dat including these new infos

```
F2TC.convert2corfile(datfilename,
                         calibration_parameters,
                         dirname_in=folder,
                        dirname_out=folder,
                        CCDCalibdict=CCDCalibdict)
corfilename = datfilename.split('.')[0] + '.cor'
fullpathcorfile = os.path.join(folder,corfilename)
```

```
nb of spots and columns in .dat file (83, 3)
file :../Examples/Ge/Ge0001.dat
containing 83 peaks
(2theta chi X Y I) written in ../Examples/Ge/Ge0001.cor
```

Create an instance of the class spotset. Initialize spots properties to data contained in .cor file

```
DataSet = ISS.spotsset()

DataSet.importdatafromfile(fullpathcorfile)
```

```
CCDcalib in readfile_cor {'dd': 69.179, 'xcen': 1050.81, 'ycen': 1115.59, 'xbet': 0.
↪104, 'xgam': -0.273, 'xpixelsize': 0.08057, 'ypixelsize': 0.08057, 'CCDLabel':
↪'sCMOS', 'framedim': [2048.0, 2048.0], 'detectordiameter': 165.00736, 'kf_direction
↪': 'Z>0', 'pixelsize': 0.08057}
CCD Detector parameters read from .cor file
CCDcalibdict {'dd': 69.179, 'xcen': 1050.81, 'ycen': 1115.59, 'xbet': 0.104, 'xgam': -
↪0.273, 'xpixelsize': 0.08057, 'ypixelsize': 0.08057, 'CCDLabel': 'sCMOS', 'framedim
↪': [2048.0, 2048.0], 'detectordiameter': 165.00736, 'kf_direction': 'Z>0',
↪'pixelsize': 0.08057}
```

```
True
```

Class methods and attributes rely on a dictionnary of spots properties. key = exprimental spot index, val = spots properties

```
[DataSet.indexed_spots_dict[k] for k in range(10)]
```

```
[[0, 78.215821, 1.638153, 1027.11, 1293.28, 70931.27, 0],
 [1, 64.329767, -20.824155, 1379.17, 1553.58, 51933.84, 0],
 [2, 68.680451, -15.358122, 1288.11, 1460.16, 22795.07, 0],
```

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```
 [3, 105.61498, 8.176187, 926.22, 872.06, 19489.69, 0],
 [4, 103.859791, 27.866566, 595.46, 876.44, 19058.79, 0],
 [5, 120.59561, -8.92066, 1183.27, 598.92, 17182.88, 0],
 [6, 60.359458, 26.483191, 626.12, 1661.28, 15825.39, 0],
 [7, 56.269853, 12.967153, 856.14, 1702.52, 15486.2, 0],
 [8, 82.072076, -35.89243, 1672.67, 1258.62, 13318.81, 0],
 [9, 83.349535, -27.458061, 1497.4, 1224.7, 13145.99, 0]]
```

```
DataSet.getUnIndexedSpotsallData()[:3]
```

```
array([[ 0.0000000e+00,  7.8215821e+01,  1.6381530e+00,  1.0271100e+03,
         1.2932800e+03,  7.0931270e+04],
       [ 1.0000000e+00,  6.4329767e+01, -2.0824155e+01,  1.3791700e+03,
         1.5535800e+03,  5.1933840e+04],
       [ 2.0000000e+00,  6.8680451e+01, -1.5358122e+01,  1.2881100e+03,
         1.4601600e+03,  2.2795070e+04]])
```

```
dict_loop = {'MATCHINGRATE_THRESHOLD_IAL': 100,
                    'MATCHINGRATE_ANGLE_TOL': 0.2,
                    'NBMAXPROBED': 6,
                    'central spots indices': [0,],
                    'AngleTolLUT': 0.5,
                    'UseIntensityWeights': False,
                    'nbSpotsToIndex':10000,
                    'list matching tol angles':[0.5,0.5,0.2,0.2],
                    'nlutmax':3,
                    'MinimumNumberMatches': 3,
                    'MinimumMatchingRate':3
                    }
grainindex=0
DataSet = ISS.spotsset()

DataSet.pixelsize = CCDCalibdict['xpixelsize']
DataSet.dim = CCDCalibdict['framedim']
DataSet.detectordiameter = CCDCalibdict['detectordiameter']
DataSet.kf_direction = CCDCalibdict['kf_direction']
DataSet.key_material = key_material
DataSet.emin = emin
DataSet.emax = emax
```

Normally we read all spots data from a .cor file

```
DataSet.importdatafromfile(fullpathcorfile)
DataSet.emin
```

```
CCDcalib in readfile_cor {'dd': 69.179, 'xcen': 1050.81, 'ycen': 1115.59, 'xbet': 0.
↪104, 'xgam': -0.273, 'xpixelsize': 0.08057, 'ypixelsize': 0.08057, 'CCDLabel':
↪'sCMOS', 'framedim': [2048.0, 2048.0], 'detectordiameter': 165.00736, 'kf_direction
↪': 'Z>0', 'pixelsize': 0.08057}
CCD Detector parameters read from .cor file
CCDcalibdict {'dd': 69.179, 'xcen': 1050.81, 'ycen': 1115.59, 'xbet': 0.104, 'xgam': -
↪0.273, 'xpixelsize': 0.08057, 'ypixelsize': 0.08057, 'CCDLabel': 'sCMOS', 'framedim
↪': [2048.0, 2048.0], 'detectordiameter': 165.00736, 'kf_direction': 'Z>0',
↪'pixelsize': 0.08057}
```

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```
5
```

but we can import a custom list of spots. For example, starting from spots a the previous .cor file

```
Gespots = RWASCII.readfile_cor(fullpathcorfile)[0]
```

```
CCDcalib in readfile_cor {'dd': 69.179, 'xcen': 1050.81, 'ycen': 1115.59, 'xbet': 0.
↪104, 'xgam': -0.273, 'xpixelsize': 0.08057, 'ypixelsize': 0.08057, 'CCDLabel':
↪'sCMOS', 'framedim': [2048.0, 2048.0], 'detectordiameter': 165.00736, 'kf_direction
↪': 'Z>0', 'pixelsize': 0.08057}
CCD Detector parameters read from .cor file
```

```
# 2theta chi X, Y Intensity of the first 7 spots
Gespots[:7,:5]
```

```
array([[ 7.82158210e+01,  1.63815300e+00,  1.02711000e+03,
         1.29328000e+03,  7.09312700e+04],
       [ 6.43297670e+01, -2.08241550e+01,  1.37917000e+03,
         1.55358000e+03,  5.19338400e+04],
       [ 6.86804510e+01, -1.53581220e+01,  1.28811000e+03,
         1.46016000e+03,  2.27950700e+04],
       [ 1.05614980e+02,  8.17618700e+00,  9.26220000e+02,
         8.72060000e+02,  1.94896900e+04],
       [ 1.03859791e+02,  2.78665660e+01,  5.95460000e+02,
         8.76440000e+02,  1.90587900e+04],
       [ 1.20595610e+02, -8.92066000e+00,  1.18327000e+03,
         5.98920000e+02,  1.71828800e+04],
       [ 6.03594580e+01,  2.64831910e+01,  6.26120000e+02,
         1.66128000e+03,  1.58253900e+04]])
```

```
tth,chi,X,Y,I=Gespots[:,:5].T
exp_data_all=np.array([tth,chi,I,X,Y])
exp_data_all.shape
```

```
(5, 83)
```

```
#select some exp spots from absolute index   (6,0,2,30,9,8,20,10,5,1,7,14)
tth_e,chi_e,X_e,Y_e,I_e = (np.take(Gespots[:,:5],(6,0,2,30,9,8,20,10,5,1,7,14),
↪axis=0)).T
exp_data=np.array([tth_e,chi_e,I_e,X_e,Y_e])
```

spots data must be imported as an array of 5 elements: 2theta, chi, Intensity, pixelX, pixelY

```
DataSet.importdata(exp_data)
DataSet.detectorparameters = calibration_parameters
DataSet.nbspots = len(exp_data[0])
DataSet.filename = 'short_'+corfilename
#DataSet.setSelectedExpSpotsData(0)
DataSet.getSelectedExpSpotsData(0)
```

```
(array([[ 6.03594580e+01,  7.82158210e+01,  6.86804510e+01,
          1.08452917e+02,  8.33495350e+01,  8.20720760e+01,
          8.17712570e+01,  9.17982210e+01,  1.20595610e+02,
          6.43297670e+01,  5.62698530e+01,  1.14942090e+02],
        [ 2.64831910e+01,  1.63815300e+00, -1.53581220e+01,
          3.77494610e+01, -2.74580610e+01, -3.58924300e+01,
          3.03824700e+01, -8.30994100e+00, -8.92066000e+00,
         -2.08241550e+01,  1.29671530e+01,  1.15295700e+01],
        [ 1.58253900e+04,  7.09312700e+04,  2.27950700e+04,
          4.40061000e+03,  1.31459900e+04,  1.33188100e+04,
          6.13787000e+03,  1.17999300e+04,  1.71828800e+04,
          5.19338400e+04,  1.54862000e+04,  1.00105200e+04]]),
 array([ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11]))
```

6.2.2 core function to index a set of spots

by defaut DataSet.getUnIndexedSpotsallData() is called

if use_file = 0, then current non indexed exp. spots will be considered for indexation

if use_file = 1, reimport data from file and reset also spots properties dictionary (i.e. with status unindexed)

```
DataSet.IndexSpotsSet(fullpathcorfile, key_material, emin, emax, dict_loop, None,
                          use_file=0, # if 1, reimport data from file and reset also␣
↪spots properties dictionary
                          IMM=False,LUT=None,n_LUT=dict_loop['nlutmax'],angletol_
↪list=dict_loop['list matching tol angles'],
                        nbGrainstoFind=1,
                      starting_grainindex=0,
                      MatchingRate_List=[1, 1, 1,1,1,1,1,1],
                        verbose=0, previousResults=None,
                        corfilename=corfilename)
```

```
self.pixelsize in IndexSpotsSet 0.08057
ResolutionAngstromLUT in IndexSpotsSet False

 Remaining nb of spots to index for grain #0 : 12


 **
start to index grain #0 of Material: Ge

**

providing new set of matrices Using Angles LUT template matching
nbspots 12
NBMAXPROBED 6
nbspots 12
set_central_spots_hkl None
Computing LUT from material data
Compute LUT for indexing Ge spots in LauePattern
Build angles LUT with latticeparameters
[ 5.657499999999999  5.657499999999999  5.657499999999999
 90.                 90.                 90.               ]
and n=3
```

```
MaxRadiusHKL False
cubicSymmetry True
Central set of exp. spotDistances from spot_index_central_list probed
self.absolute_index [ 0  1  2  3  4  5  6  7  8  9 10 11]
spot_index_central_list [0]
[0]
LUT is not None when entering getOrientMatrices()
set_central_spots_hkl None
set_central_spots_hkl_list [None]
cubicSymmetry True
LUT_tol_angle 0.5
---***-----------------------------------------------*
Calculating all possible matrices from exp spot #0 and the 5 other(s)
hkl in getOrientMatrices None <class 'NoneType'>
using LUTcubic
LUTcubic is None for k_centspot_index 0 in getOrientMatrices()
hkl1 in matrices_from_onespot_hkl() [[1 0 0]
 [1 1 0]
 [1 1 1]
 [2 1 0]
 [2 1 1]
 [2 2 1]
 [3 1 0]
 [3 1 1]
 [3 2 1]
 [3 2 2]
 [3 3 1]
 [3 3 2]]
Computing hkl2 list for specific or cubic LUT in matrices_from_onespot_hkl()
Calculating LUT in PlanePairs_from2sets()
Looking up planes pairs in LUT from exp. spots (0, 1):
Looking up planes pairs in LUT from exp. spots (0, 2):
Looking up planes pairs in LUT from exp. spots (0, 3):
Looking up planes pairs in LUT from exp. spots (0, 4):
Looking up planes pairs in LUT from exp. spots (0, 5):
calculating matching rates of solutions for exp. spots [0, 1]
calculating matching rates of solutions for exp. spots [0, 2]
calculating matching rates of solutions for exp. spots [0, 3]
calculating matching rates of solutions for exp. spots [0, 4]


return best matrix and matching scores for the one central_spot

----------------------------------------
results:
matrix:                                              matching results
[-0.211852735694566  0.092255643652867 -0.972937466948891]        res: [20.0,␣
↪162.0] 0.014 12.35
[-0.775856536468367  0.58951816141498   0.22475536073965 ]        spot␣
↪indices [0 1]
[ 0.594300563948835  0.802473664571131 -0.053318452339475]        planes [[1.
↪0, 3.0, 2.0], [1.0, 1.0, 1.0]]

Number of matrices found (nb_sol):  1
```

```
set_central_spots_hkl in FindOrientMatrices None

----------------------------------------
results:
matrix:                                              matching results
[-0.211852735694566  0.092255643652867 -0.972937466948891]        res: [20.0,␣
↪162.0] 0.014 12.35
[-0.775856536468367  0.58951816141498   0.22475536073965 ]        spot␣
↪indices [0 1]
[ 0.594300563948835  0.802473664571131 -0.053318452339475]        planes [[1.
↪0, 3.0, 2.0], [1.0, 1.0, 1.0]]

Nb of potential orientation matrice(s) UB found: 1
[array([[-0.211852735694566,  0.092255643652867, -0.972937466948891],
       [-0.775856536468367,  0.58951816141498 ,  0.22475536073965 ],
       [ 0.594300563948835,  0.802473664571131, -0.053318452339475]])]
Nb of potential UBs  1

Working with a new stack of orientation matrices
MATCHINGRATE_THRESHOLD_IAL= 100.0
has not been reached! All potential solutions have been calculated
taking the first one only.
bestUB object <LaueTools.indexingSpotsSet.OrientMatrix object at␣
↪0x7fb8ec7ddc50>


---------------refining grain orientation and strain #0-----------------


 refining grain #0 step -----0

bestUB <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7fb8ec7ddc50>
True it is an OrientMatrix object
Orientation <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7fb8ec7ddc50>
matrix [[-0.211852735694566  0.092255643652867 -0.972937466948891]
 [-0.775856536468367  0.58951816141498   0.22475536073965 ]
 [ 0.594300563948835  0.802473664571131 -0.053318452339475]]
*nb of selected spots in AssignHKL*** 12
UBOrientMatrix [[-0.211852735694566  0.092255643652867 -0.972937466948891]
 [-0.775856536468367  0.58951816141498   0.22475536073965 ]
 [ 0.594300563948835  0.802473664571131 -0.053318452339475]]
For angular tolerance 0.50 deg
Nb of pairs found / nb total of expected spots: 12/176
Matching Rate : 6.82
Nb missing reflections: 164

grain #0 : 12 links to simulated spots have been found
*********mean pixel deviation    0.560750282710606     ******
Initial residues [0.053680370172309 0.013739858524874 0.921977335411896 0.
↪403270956234836
 0.919825854310187 0.785969463406447 0.565019172757509 1.127873079813964
 0.363514793614926 0.412635402450867 0.711008521607465 0.450488584221994]
----------------------------------------------------
```

```
**********************
first error with initial values of: ['b/a', 'c/a', 'a12', 'a13', 'a23',␣
↪'theta1', 'theta2', 'theta3']

**********************

*********mean pixel deviation    0.560750282710606     ******


**********************
Fitting parameters:   ['b/a', 'c/a', 'a12', 'a13', 'a23', 'theta1', 'theta2',␣
↪'theta3']

**********************

With initial values [1. 1. 0. 0. 0. 0. 0. 0.]
code results 1
nb iterations 1767
mesg Both actual and predicted relative reductions in the sum of squares
  are at most 0.000000
strain_sol [ 1.001128981010799e+00  9.993806401299155e-01  8.449040381845989e-
↪04
 -8.486913595751131e-04  3.520626401662759e-04 -2.714612741167435e-02
  3.054889720130747e-02  5.311773668297186e-02]


 **********  End of Fitting  -  Final errors  **************


*********mean pixel deviation    0.3158807195732847     ******
devstrain, lattice_parameter_direct_strain [[ 0.000159671589578 -0.
↪000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]] [ 5.
↪657424223234738  5.651101185787196  5.661104877237695
 90.01741959362538  89.9544419036642   90.04747664598754 ]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.657499999999999  5.651176877860324  5.
↪661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
devstrain1, lattice_parameter_direct_strain1 [[ 0.000159671589578 -0.
↪000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]] [ 5.
↪657499999999999  5.651176877860324  5.661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[-1.339403716515974e-05 -4.138432477238585e-04  3.
↪978226745502020e-04]
 [-4.138432477238585e-04 -1.131375039302607e-03 -1.517818975573709e-04]
 [ 3.978226745502020e-04 -1.517818975573709e-04  6.255721962393768e-04]]
```

```
deviatoric strain [[ 0.000159671589578 -0.000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[-1.339403716515974e-05 -4.138432477238585e-04  3.
↪978226745502020e-04]
 [-4.138432477238585e-04 -1.131375039302607e-03 -1.517818975573709e-04]
 [ 3.978226745502020e-04 -1.517818975573709e-04  6.255721962393768e-04]]
deviatoric strain [[ 0.000159671589578 -0.000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.657499999999999  5.651176877860324  5.
↪661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
final lattice_parameters [ 5.657499999999999  5.651176877860324  5.
↪661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
UB and strain refinement completed
True it is an OrientMatrix object
Orientation <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7fb8c98baa20>
matrix [[-0.211415207301911  0.091252946262469 -0.97230572627369 ]
 [-0.77573594328912   0.590041596352251  0.224552051799525]
 [ 0.594613709497768  0.803610914885283 -0.054088075690982]]
*nb of selected spots in AssignHKL*** 12
UBOrientMatrix [[-0.211415207301911  0.091252946262469 -0.97230572627369 ]
 [-0.77573594328912   0.590041596352251  0.224552051799525]
 [ 0.594613709497768  0.803610914885283 -0.054088075690982]]
For angular tolerance 0.50 deg
Nb of pairs found / nb total of expected spots: 12/177
Matching Rate : 6.78
Nb missing reflections: 165

grain #0 : 12 links to simulated spots have been found
GoodRefinement condition is  True
nb_updates 12 compared to 6


 refining grain #0 step -----1

bestUB <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7fb8ec7ddc50>
True it is an OrientMatrix object
Orientation <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7fb8ec7ddc50>
matrix [[-0.211852735694566  0.092255643652867 -0.972937466948891]
 [-0.775856536468367  0.58951816141498   0.224755360739651 ]
 [ 0.594300563948835  0.802473664571131 -0.053318452339475]]
*nb of selected spots in AssignHKL*** 12
UBOrientMatrix [[-0.211852735694566  0.092255643652867 -0.972937466948891]
 [-0.775856536468367  0.58951816141498   0.224755360739651 ]
 [ 0.594300563948835  0.802473664571131 -0.053318452339475]]
For angular tolerance 0.50 deg
Nb of pairs found / nb total of expected spots: 12/176
Matching Rate : 6.82
```

```
Nb missing reflections: 164

grain #0 : 12 links to simulated spots have been found
*********mean pixel deviation    0.560750282710606     ******
Initial residues [0.053680370172309 0.013739858524874 0.921977335411896 0.
↪403270956234836
 0.919825854310187 0.785969463406447 0.565019172757509 1.127873079813964
 0.363514793614926 0.412635402450867 0.711008521607465 0.450488584221994]
--------------------------------------------------



**********************
first error with initial values of: ['b/a', 'c/a', 'a12', 'a13', 'a23',␣
↪'theta1', 'theta2', 'theta3']

**********************

*********mean pixel deviation    0.560750282710606     ******


**********************
Fitting parameters:   ['b/a', 'c/a', 'a12', 'a13', 'a23', 'theta1', 'theta2',␣
↪'theta3']

**********************

With initial values [1. 1. 0. 0. 0. 0. 0. 0.]
code results 1
nb iterations 1767
mesg Both actual and predicted relative reductions in the sum of squares
  are at most 0.000000
strain_sol [ 1.001128981010799e+00  9.993806401299155e-01  8.449040381845989e-
↪04
 -8.486913595751131e-04  3.520626401662759e-04 -2.714612741167435e-02
  3.054889720130747e-02  5.311773668297186e-02]


 **********  End of Fitting  -  Final errors  **************


*********mean pixel deviation    0.3158807195732847     ******
devstrain, lattice_parameter_direct_strain [[ 0.000159671589578 -0.
↪000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]] [ 5.
↪657424223234738  5.651101185787196  5.661104877237695
 90.01741959362538  89.9544419036642   90.04747664598754 ]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.657499999999999  5.651176877860324  5.
↪661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
devstrain1, lattice_parameter_direct_strain1 [[ 0.000159671589578 -0.
```

```
 ↪000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]] [ 5.
 ↪657499999999999  5.651176877860324  5.661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[-1.339403716515974e-05 -4.138432477238585e-04  3.
 ↪978226745502020e-04]
 [-4.138432477238585e-04 -1.131375039302607e-03 -1.517818975573709e-04]
 [ 3.978226745502020e-04 -1.517818975573709e-04  6.255721962393768e-04]]
deviatoric strain [[ 0.000159671589578 -0.000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[-1.339403716515974e-05 -4.138432477238585e-04  3.
 ↪978226745502020e-04]
 [-4.138432477238585e-04 -1.131375039302607e-03 -1.517818975573709e-04]
 [ 3.978226745502020e-04 -1.517818975573709e-04  6.255721962393768e-04]]
deviatoric strain [[ 0.000159671589578 -0.000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
 ↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.657499999999999  5.651176877860324  5.
 ↪661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
final lattice_parameters [ 5.657499999999999  5.651176877860324  5.
 ↪661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
UB and strain refinement completed
True it is an OrientMatrix object
Orientation <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7fb8c98ba9b0>
matrix [[-0.211415207301911  0.091252946262469 -0.97230572627369 ]
 [-0.77573594328912   0.590041596352251  0.224552051799525]
 [ 0.594613709497768  0.803610914885283 -0.054088075690982]]
*nb of selected spots in AssignHKL*** 12
UBOrientMatrix [[-0.211415207301911  0.091252946262469 -0.97230572627369 ]
 [-0.77573594328912   0.590041596352251  0.224552051799525]
 [ 0.594613709497768  0.803610914885283 -0.054088075690982]]
For angular tolerance 0.50 deg
Nb of pairs found / nb total of expected spots: 12/177
Matching Rate : 6.78
Nb missing reflections: 165

grain #0 : 12 links to simulated spots have been found
GoodRefinement condition is  True
nb_updates 12 compared to 6


 refining grain #0 step -----2

bestUB <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7fb8ec7ddc50>
True it is an OrientMatrix object
Orientation <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7fb8ec7ddc50>
```

```
matrix [[-0.211852735694566  0.092255643652867 -0.972937466948891]
 [-0.775856536468367  0.58951816141498   0.22475536073965 ]
 [ 0.594300563948835  0.802473664571131 -0.053318452339475]]
*nb of selected spots in AssignHKL*** 12
UBOrientMatrix [[-0.211852735694566  0.092255643652867 -0.972937466948891]
 [-0.775856536468367  0.58951816141498   0.22475536073965 ]
 [ 0.594300563948835  0.802473664571131 -0.053318452339475]]
For angular tolerance 0.20 deg
Nb of pairs found / nb total of expected spots: 12/176
Matching Rate : 6.82
Nb missing reflections: 164

grain #0 : 12 links to simulated spots have been found
*********mean pixel deviation    0.560750282710606     ******
Initial residues [0.053680370172309 0.013739858524874 0.921977335411896 0.
↪403270956234836
 0.919825854310187 0.785969463406447 0.565019172757509 1.127873079813964
 0.363514793614926 0.412635402450867 0.711008521607465 0.450488584221994]
--------------------------------------------------



**********************
first error with initial values of: ['b/a', 'c/a', 'a12', 'a13', 'a23',␣
↪'theta1', 'theta2', 'theta3']

**********************

*********mean pixel deviation    0.560750282710606     ******


**********************
Fitting parameters:   ['b/a', 'c/a', 'a12', 'a13', 'a23', 'theta1', 'theta2',␣
↪'theta3']

**********************

With initial values [1. 1. 0. 0. 0. 0. 0. 0.]
code results 1
nb iterations 1767
mesg Both actual and predicted relative reductions in the sum of squares
  are at most 0.000000
strain_sol [ 1.001128981010799e+00  9.993806401299155e-01  8.449040381845989e-
↪04
 -8.486913595751131e-04  3.520626401662759e-04 -2.714612741167435e-02
  3.054889720130747e-02  5.311773668297186e-02]


 **********  End of Fitting  -  Final errors  **************


*********mean pixel deviation    0.3158807195732847     ******
devstrain, lattice_parameter_direct_strain [[ 0.000159671589578 -0.
↪000413843247724  0.00039782267455 ]
```

```
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]] [ 5.
↪657424223234738  5.651101185787196  5.661104877237695
 90.01741959362538  89.9544419036642   90.04747664598754 ]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.657499999999999  5.651176877860324  5.
↪661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
devstrain1, lattice_parameter_direct_strain1 [[ 0.000159671589578 -0.
↪000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]] [ 5.
↪657499999999999  5.651176877860324  5.661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[-1.339403716515974e-05 -4.138432477238585e-04  3.
↪978226745502020e-04]
 [-4.138432477238585e-04 -1.131375039302607e-03 -1.517818975573709e-04]
 [ 3.978226745502020e-04 -1.517818975573709e-04  6.255721962393768e-04]]
deviatoric strain [[ 0.000159671589578 -0.000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[-1.339403716515974e-05 -4.138432477238585e-04  3.
↪978226745502020e-04]
 [-4.138432477238585e-04 -1.131375039302607e-03 -1.517818975573709e-04]
 [ 3.978226745502020e-04 -1.517818975573709e-04  6.255721962393768e-04]]
deviatoric strain [[ 0.000159671589578 -0.000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.657499999999999  5.651176877860324  5.
↪661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
final lattice_parameters [ 5.657499999999999  5.651176877860324  5.
↪661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
UB and strain refinement completed
True it is an OrientMatrix object
Orientation <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7fb8cf573a90>
matrix [[-0.211415207301911  0.091252946262469 -0.97230572627369 ]
 [-0.77573594328912   0.590041596352251  0.224552051799525]
 [ 0.594613709497768  0.803610914885283 -0.054088075690982]]
*nb of selected spots in AssignHKL*** 12
UBOrientMatrix [[-0.211415207301911  0.091252946262469 -0.97230572627369 ]
 [-0.77573594328912   0.590041596352251  0.224552051799525]
 [ 0.594613709497768  0.803610914885283 -0.054088075690982]]
For angular tolerance 0.20 deg
Nb of pairs found / nb total of expected spots: 12/177
Matching Rate : 6.78
Nb missing reflections: 165
```

```
grain #0 : 12 links to simulated spots have been found
GoodRefinement condition is  True
nb_updates 12 compared to 6


 refining grain #0 step -----3

bestUB <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7fb8ec7ddc50>
True it is an OrientMatrix object
Orientation <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7fb8ec7ddc50>
matrix [[-0.211852735694566  0.092255643652867 -0.972937466948891]
 [-0.775856536468367  0.58951816141498   0.22475536073965 ]
 [ 0.594300563948835  0.802473664571131 -0.053318452339475]]
*nb of selected spots in AssignHKL*** 12
UBOrientMatrix [[-0.211852735694566  0.092255643652867 -0.972937466948891]
 [-0.775856536468367  0.58951816141498   0.22475536073965 ]
 [ 0.594300563948835  0.802473664571131 -0.053318452339475]]
For angular tolerance 0.20 deg
Nb of pairs found / nb total of expected spots: 12/176
Matching Rate : 6.82
Nb missing reflections: 164

grain #0 : 12 links to simulated spots have been found
*********mean pixel deviation    0.560750282710606     ******
Initial residues [0.053680370172309 0.013739858524874 0.921977335411896 0.
↪403270956234836
 0.919825854310187 0.785969463406447 0.565019172757509 1.127873079813964
 0.363514793614926 0.412635402450867 0.711008521607465 0.450488584221994]
--------------------------------------------------



**********************
first error with initial values of: ['b/a', 'c/a', 'a12', 'a13', 'a23',␣
↪'theta1', 'theta2', 'theta3']

**********************

*********mean pixel deviation    0.560750282710606     ******


**********************
Fitting parameters:   ['b/a', 'c/a', 'a12', 'a13', 'a23', 'theta1', 'theta2',␣
↪'theta3']

**********************

With initial values [1. 1. 0. 0. 0. 0. 0. 0.]
code results 1
nb iterations 1767
mesg Both actual and predicted relative reductions in the sum of squares
  are at most 0.000000
strain_sol [ 1.001128981010799e+00  9.993806401299155e-01  8.449040381845989e-
↪04
```

```
 -8.486913595751131e-04  3.520626401662759e-04 -2.714612741167435e-02
  3.054889720130747e-02  5.311773668297186e-02]


 ********** End of Fitting - Final errors **************


**********mean pixel deviation    0.3158807195732847     ******
devstrain, lattice_parameter_direct_strain [[ 0.000159671589578 -0.
↪000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]] [ 5.
↪657424223234738  5.651101185787196  5.661104877237695
 90.01741959362538  89.9544419036642   90.04747664598754 ]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.657499999999999  5.651176877860324  5.
↪661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
devstrain1, lattice_parameter_direct_strain1 [[ 0.000159671589578 -0.
↪000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]] [ 5.
↪657499999999999  5.651176877860324  5.661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[-1.339403716515974e-05 -4.138432477238585e-04  3.
↪978226745502020e-04]
 [-4.138432477238585e-04 -1.131375039302607e-03 -1.517818975573709e-04]
 [ 3.978226745502020e-04 -1.517818975573709e-04  6.255721962393768e-04]]
deviatoric strain [[ 0.000159671589578 -0.000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[-1.339403716515974e-05 -4.138432477238585e-04  3.
↪978226745502020e-04]
 [-4.138432477238585e-04 -1.131375039302607e-03 -1.517818975573709e-04]
 [ 3.978226745502020e-04 -1.517818975573709e-04  6.255721962393768e-04]]
deviatoric strain [[ 0.000159671589578 -0.000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.657499999999999  5.651176877860324  5.
↪661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
final lattice_parameters [ 5.657499999999999  5.651176877860324  5.
↪661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
UB and strain refinement completed
True it is an OrientMatrix object
Orientation <LaueTools.indexingSpotsSet.OrientMatrix object at 0x7fb8ec7bc128>
matrix [[-0.211415207301911  0.091252946262469 -0.97230572627369 ]
 [-0.77573594328912   0.590041596352251  0.224552051799525]
```

```
 [ 0.594613709497768  0.803610914885283 -0.054088075690982]]
*nb of selected spots in AssignHKL*** 12
UBOrientMatrix [[-0.211415207301911  0.091252946262469 -0.97230572627369 ]
 [-0.77573594328912   0.590041596352251  0.224552051799525]
 [ 0.594613709497768  0.803610914885283 -0.054088075690982]]
For angular tolerance 0.20 deg
Nb of pairs found / nb total of expected spots: 12/177
Matching Rate : 6.78
Nb missing reflections: 165

grain #0 : 12 links to simulated spots have been found
GoodRefinement condition is  True
nb_updates 12 compared to 6

-------------------------------------------
indexing completed for grain #0 with matching rate 6.78
-------------------------------------------

transform matrix to matrix with lowest Euler Angles
start
 [[-0.211415207301911  0.091252946262469 -0.97230572627369 ]
 [-0.77573594328912   0.590041596352251  0.224552051799525]
 [ 0.594613709497768  0.803610914885283 -0.054088075690982]]
final
 [[ 0.97230572627369   0.211415207301911  0.091252946262469]
 [-0.224552051799525  0.77573594328912   0.590041596352251]
 [ 0.054088075690982 -0.594613709497768  0.803610914885283]]
hkl [[2. 6. 4.]
 [3. 3. 3.]
 [5. 3. 3.]
 [1. 3. 5.]
 [6. 2. 4.]
 [5. 1. 3.]
 [1. 3. 3.]
 [6. 4. 6.]
 [4. 2. 6.]
 [4. 2. 2.]
 [3. 5. 3.]
 [2. 2. 4.]]
new hkl (min euler angles) [[-4. -2.  6.]
 [-3. -3.  3.]
 [-3. -5.  3.]
 [-5. -1.  3.]
 [-4. -6.  2.]
 [-3. -5.  1.]
 [-3. -1.  3.]
 [-6. -6.  4.]
 [-6. -4.  2.]
 [-2. -4.  2.]
 [-3. -3.  5.]
 [-4. -2.  2.]]
UB before [[-0.211415207301911  0.091252946262469 -0.97230572627369 ]
 [-0.77573594328912   0.590041596352251  0.224552051799525]
 [ 0.594613709497768  0.803610914885283 -0.054088075690982]]
```

```
new UB (min euler angles) [[ 0.97230572627369   0.211415207301911  0.
↪091252946262469]
 [-0.224552051799525  0.77573594328912   0.590041596352251]
 [ 0.054088075690982 -0.594613709497768  0.803610914885283]]
writing fit file -------------------------
for grainindex= 0
self.dict_grain_matrix[grain_index] [[ 0.97230572627369   0.211415207301911 ␣
↪0.091252946262469]
 [-0.224552051799525  0.77573594328912   0.590041596352251]
 [ 0.054088075690982 -0.594613709497768  0.803610914885283]]
self.refinedUBmatrix [[-0.211415207301911  0.091252946262469 -0.
↪97230572627369 ]
 [-0.77573594328912   0.590041596352251  0.224552051799525]
 [ 0.594613709497768  0.803610914885283 -0.054088075690982]]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[-1.339403716515974e-05 -4.138432477238585e-04  3.
↪978226745502020e-04]
 [-4.138432477238585e-04 -1.131375039302607e-03 -1.517818975573709e-04]
 [ 3.978226745502020e-04 -1.517818975573709e-04  6.255721962393768e-04]]
deviatoric strain [[ 0.000159671589578 -0.000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]]
new UBs matrix in q= UBs G (s for strain)
strain_direct [[-1.339403716515974e-05 -4.138432477238585e-04  3.
↪978226745502020e-04]
 [-4.138432477238585e-04 -1.131375039302607e-03 -1.517818975573709e-04]
 [ 3.978226745502020e-04 -1.517818975573709e-04  6.255721962393768e-04]]
deviatoric strain [[ 0.000159671589578 -0.000413843247724  0.00039782267455 ]
 [-0.000413843247724 -0.00095830941256  -0.000151781897557]
 [ 0.00039782267455  -0.000151781897557  0.000798637822982]]
For comparison: a,b,c are rescaled with respect to the reference value of a =␣
↪5.657500 Angstroms
lattice_parameter_direct_strain [ 5.657499999999999  5.651176877860324  5.
↪661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
final lattice_parameters [ 5.657499999999999  5.651176877860324  5.
↪661180703302433
 90.01741959362538  89.9544419036642   90.04747664598754 ]
File : Ge0001_g0.fit written in /home/micha/LaueToolsPy3/LaueTools/notebooks
Experimental experimental spots indices which are not indexed []
Missing reflections grainindex is -100 for indexed grainindex 0
within angular tolerance 0.500

 Remaining nb of spots to index for grain #1 : 0

12 spots have been indexed over 12
indexing rate is --- : 100.0 percents
indexation of short_Ge0001.cor is completed
for the 1 grain(s) that has(ve) been indexed as requested
Leaving Index and Refine procedures...
```

```
index_grain_retrieve=0
print("number of indexed spots", len(DataSet.getallIndexedSpotsallData()[index_grain_
↪retrieve]))
```

```
number of indexed spots 12
```

6.2.3 Results of indexation can be found in attributes or through methods

```
spotsdata=DataSet.getSummaryallData()
print("first 2 indexed spots properties\n")
print('#spot  #grain 2theta chi X Y I h k l Energy')
print(spotsdata[:2])
```

```
first 2 indexed spots properties

#spot  #grain 2theta chi X Y I h k l Energy
[[ 0.000000000000000e+00  0.000000000000000e+00  6.035945800000000e+01
   2.648319100000000e+01  6.261200000000000e+02  1.661280000000000e+03
   1.582539000000000e+04 -4.000000000000000e+00 -2.000000000000000e+00
   6.000000000000000e+00  1.632366988464985e+01]
 [ 1.000000000000000e+00  0.000000000000000e+00  7.821582100000001e+01
   1.638153000000000e+00  1.027110000000000e+03  1.293280000000000e+03
   7.093127000000000e+04 -3.000000000000000e+00 -3.000000000000000e+00
   3.000000000000000e+00  9.031851548397370e+00]]
```

```
print('#grain  : [Npairs = Nb pairs with tolerance angle %.4f, 100*Npairs/Ndirections␣
↪theo.]'%dict_loop['list matching tol angles'][-1])
DataSet.dict_grain_matching_rate
```

```
#grain  : [Npairs = Nb pairs with tolerance angle 0.2000, 100*Npairs/Ndirections theo.
↪]
```

```
{0: [12, 6.779661016949152]}
```

```
print("#grain  : deviatoric strain")
DataSet.dict_grain_devstrain
```

```
#grain  : deviatoric strain
```

```
{0: array([[ 0.000159671589578, -0.000413843247724,  0.00039782267455 ],
        [-0.000413843247724, -0.00095830941256 , -0.000151781897557],
        [ 0.00039782267455 , -0.000151781897557,  0.000798637822982]])}
```

```
#RefinedUB= DataSet.dict_grain_matrix
print("#grain  : refined UB matrix")
DataSet.dict_grain_matrix
```

```
#grain  : refined UB matrix
```

```
{0: array([[ 0.97230572627369 ,  0.211415207301911,  0.091252946262469],
        [-0.224552051799525,  0.77573594328912 ,  0.590041596352251],
        [ 0.054088075690982, -0.594613709497768,  0.803610914885283]])}
```

```
print([DataSet.indexed_spots_dict[k] for k in range(10)])
```

```
[[0, 60.359458, 26.483191, 626.12, 1661.28, 15825.39, array([-4., -2.,  6.]), 16.
↪323669884649853, 0, 1], [1, 78.215821, 1.638153, 1027.11, 1293.28, 70931.27,␣
↪array([-3., -3.,  3.]), 9.03185154839737, 0, 1], [2, 68.680451, -15.358122, 1288.11,
↪ 1460.16, 22795.07, array([-3., -5.,  3.]), 12.73794897550435, 0, 1], [3, 108.
↪452917, 37.749461, 383.77, 754.58, 4400.61, array([-5., -1.,  3.]), 7.
↪989738078276174, 0, 1], [4, 83.349535, -27.458061, 1497.4, 1224.7, 13145.99,␣
↪array([-4., -6.,  2.]), 12.327936233758937, 0, 1], [5, 82.072076, -35.89243, 1672.
↪67, 1258.62, 13318.81, array([-3., -5.,  1.]), 9.870774398536632, 0, 1], [6, 81.
↪771257, 30.38247, 548.25, 1260.32, 6137.87, array([-3., -1.,  3.]), 7.
↪2986772558942405, 0, 1], [7, 91.798221, -8.309941, 1176.09, 1086.19, 11799.93,␣
↪array([-6., -6.,  4.]), 14.309911950813975, 0, 1], [8, 120.59561, -8.92066, 1183.27,
↪ 598.92, 17182.88, array([-6., -4.,  2.]), 9.435284238042113, 0, 1], [9, 64.329767,␣
↪-20.824155, 1379.17, 1553.58, 51933.84, array([-2., -4.,  2.]), 10.087272916663885,␣
↪0, 1]]
```

CHAPTER

SEVEN

LAUETOOLS MODULES

7.1 Browse Modules and Functions

- genindex
- modindex

7.2 Modules for Laue Pattern Simulation

The following modules are used to compute Laue pattern from grain (or crystal) structural parameters and 2D plane detector geometry:

- *CrystalParameters.py* defines structural parameters describing the crystal. It includes orientation matrix and strain operators.
- *lauecore.py* contains the core procedures to compute all Laue spots properties.
- *LaueGeometry.py* handles the 2D plane geometry set by the detector position and orientation with respect to sample and incoming direction.
- *multigrainsSimulator.py* allows to simulate an assembly of grains, some of them according to a distribution of grains. This module is called by the graphical user interface (LaueSimulatorGUI) which provides all arguments in an intuitive way.

7.2.1 CrystalParameters

This module belong to LaueTools package. It gathers procedures to define crystal lattice parameters and strain calculations

Main authors are JS Micha, O. Robach, S. Tardif June 2019

LaueTools.CrystalParameters.**GrainParameter_from_Material**(*key_material, dictmaterials={'Al': ['Al', [4.05, 4.05, 4.05, 90, 90, 90], 'fcc'], 'Al2Cu': ['Al2Cu', [6.063, 6.063, 4.872, 90, 90, 90], 'no'], 'Al2O3': ['Al2O3', [4.785, 4.785, 12.991, 90, 90, 120], 'Al2O3'], 'Al2O3_all': ['Al2O3_all', [4.785, 4.785, 12.991, 90, 90, 120], 'no'], 'AlN': ['AlN', [3.11, 3.11, 4.98, 90.0, 90.0, 120.0], 'wurtzite'], 'Au': ['Au', [4.078, 4.078, 4.078, 90, 90, 90], 'fcc'], 'CCDL1949': ['CCDL1949', [9.89, 17.85, 5.31, 90, 107.5, 90], 'h+k=2n'], 'CdHgTe': ['CdHgTe', [6.46678, 6.46678, 6.46678, 90, 90, 90], 'dia'], 'CdHgTe_fcc': ['CdHgTe_fcc', [6.46678, 6.46678, 6.46678, 90, 90, 90], 'fcc'], 'CdTe': ['CdTe', [6.487, 6.487, 6.487, 90, 90, 90], 'fcc'], 'CdTeDiagB': ['CdTeDiagB', [4.5721, 7.9191, 11.1993, 90, 90, 90], 'no'], 'Crocidolite': ['Crocidolite', [9.811, 18.013, 5.326, 90, 103.68, 90], 'no'], 'Crocidolite_2': ['Crocidolite_2', [9.76, 17.93, 5.35, 90, 103.6, 90], 'no'], 'Crocidolite_2_72deg': ['Crocidolite_2', [9.76, 17.93, 5.35, 90, 76.4, 90], 'no'], 'Crocidolite_small': ['Crocidolite_small', [3.2533333333333334, 5.976666666666667, 1.7833333333333332, 90, 103.6, 90], 'no'], 'Crocidolite_whittaker_1949': ['Crocidolite_whittaker_1949', [9.89, 17.85, 5.31, 90, 107.5, 90], 'no'], 'Cu': ['Cu', [3.6, 3.6, 3.6, 90, 90, 90], 'fcc'],*

create grain parameters list for the Laue pattern simulation

Can handle material defined in dictionary by four elements instead of 6 lattice parameters

Parameters **key_material** (*string*) – material or structure label

Returns grain (4 elements list), contains_U (boolean)

LaueTools.CrystalParameters.**Prepare_Grain**(*key_material, OrientMatrix, force_extinction=None, dictmaterials={'Al': ['Al', [4.05, 4.05, 4.05, 90, 90, 90], 'fcc'], 'Al2Cu': ['Al2Cu', [6.063, 6.063, 4.872, 90, 90, 90], 'no'], 'Al2O3': ['Al2O3', [4.785, 4.785, 12.991, 90, 90, 120], 'Al2O3'], 'Al2O3_all': ['Al2O3_all', [4.785, 4.785, 12.991, 90, 90, 120], 'no'], 'AlN': ['AlN', [3.11, 3.11, 4.98, 90.0, 90.0, 120.0], 'wurtzite'], 'Au': ['Au', [4.078, 4.078, 4.078, 90, 90, 90], 'fcc'], 'CCDL1949': ['CCDL1949', [9.89, 17.85, 5.31, 90, 107.5, 90], 'h+k=2n'], 'CdHgTe': ['CdHgTe', [6.46678, 6.46678, 6.46678, 90, 90, 90], 'dia'], 'CdHgTe_fcc': ['CdHgTe_fcc', [6.46678, 6.46678, 6.46678, 90, 90, 90], 'fcc'], 'CdTe': ['CdTe', [6.487, 6.487, 6.487, 90, 90, 90], 'fcc'], 'CdTeDiagB': ['CdTeDiagB', [4.5721, 7.9191, 11.1993, 90, 90, 90], 'no'], 'Crocidolite': ['Crocidolite', [9.811, 18.013, 5.326, 90, 103.68, 90], 'no'], 'Crocidolite_2': ['Crocidolite_2', [9.76, 17.93, 5.35, 90, 103.6, 90], 'no'], 'Crocidolite_2_72deg': ['Crocidolite_2', [9.76, 17.93, 5.35, 90, 76.4, 90], 'no'], 'Crocidolite_small': ['Crocidolite_small', [3.2533333333333334, 5.976666666666667, 1.7833333333333332, 90, 103.6, 90], 'no'], 'Crocidolite_whittaker_1949': ['Crocidolite_whittaker_1949', [9.89, 17.85, 5.31, 90, 107.5, 90], 'no'], 'Cu': ['Cu', [3.6, 3.6, 3.6, 90, 90, 90], 'fcc'], 'Cu6Sn5_monoclinic': ['Cu6Sn5_monoclinic', [11.02, 7.28, 9.827, 90, 98.84, 90], 'no'], 'Cu6Sn5_tetra': ['Cu6Sn5_tetra', [3.608, 3.608, 5.037, 90, 90, 90], 'no'], 'DIA': ['DIA', [5.0, 5.0, 5.0, 90, 90, 90], 'dia'], 'DIAs': ['DIAs', [3.56683, 3.56683, 3.56683, 90, 90, 90], 'dia'], 'DarinaMolecule': ['DarinaMolecule', [9.4254, 13.5004, 13.8241, 61.83, 84.555, 75.231], 'no'], 'FCC': ['FCC', [5.0, 5.0, 5.0, 90, 90, 90], 'fcc'], 'Fe': ['Fe', [2.856, 2.856, 2.856, 90, 90, 90], 'bcc'], 'Fe2Ta': ['Fe2Ta', [4.83, 4.83, 0.788, 90, 90, 120], 'no'], 'FeAl': ['FeAl', [5.871, 5.871, 5.871, 90, 90, 90], 'fcc'], 'GaAs': ['GaAs', [5.65325, 5.65325, 5.65325, 90, 90, 90], 'dia'], 'GaN': ['GaN', [3.189, 3.189, 5.185, 90, 90, 120], 'wurtzite'], 'GaN_all': ['GaN_all', [3.189, 3.189, 5.185, 90, 90, 120], 'no'], 'Ge': ['Ge', [5.6575, 5.6575, 5.6575, 90, 90, 90], 'dia'], 'Ge_compressedhydro': ['Ge_compressedhydro', [5.64, 5.64, 5.64, 90, 90, 90.0], 'dia'], 'Ge_s': ['Ge_s', [5.6575, 5.6575, 5.6575, 90, 90, 89.5], 'dia'], 'Getest': ['Getest', [5.6575, 5.6575, 5.6574, 90, 90, 90], 'dia'], 'Hematite': ['Hematite', [5.03459, 5.03459, 13.7533, 90, 90, 120], 'no'], 'In': ['In', [3.2517, 3.2517, 4.9459, 90, 90, 90], 'h+k+l=2n'], 'InGaN': ['InGaN', [3.3609999999999998, 3.3609999999999998, 5.439, 90, 90, 120], 'wurtzite'], 'InN': ['InN', [3.533, 3.533, 5.693, 90, 90, 120], 'wurtzite'],*

Constructor of the grain (crystal) parameters for Laue pattern simulation

if in key_material definition (see dict_Materials) orient matrix is missing (i.e. only lattice parameter are input)

Parameters **key_material** (*str*) – material label

then list parameter will consider the provided value of the optional OrientMatrix argument

Parameters **force_extinction** (*str*) – None, use default extinction rules, otherwise use other extinction correspondoing to the label

LaueTools.CrystalParameters.**AngleBetweenNormals**(*HKL1s*, *HKL2s*, *Gstar*)

compute pairwise angles (in degrees) between reflections or lattice plane normals of two sets according to unit cell metrics Gstar

Parameters

- **HKL1s** – list of [H1,K1,L1]
- **HKL2s** – list of [H2,K2,L2]
- **Gstar** – 3*3 matrix corresponding to reciprocal metric tensor of unit cell (as provided by Gstar_from_directlatticeparams())

Returns array of pairwise angles between reflections

LaueTools.CrystalParameters.**FilterHarmonics_2**(*hkl*, *return_indices_toremove=0*)

keep only hkl 3d vectors that are representative of direction nh,nk,nl for any h,k,l signed integers

It removes only parallel vector but KEEPs antiparallel vectors (vec , -n vec) with n>0

Parameters

- **hkl** – array of 3d hkl indices
- **return_indices_toremove** – 1, returns indices of element in hkl that have been removed

LaueTools.CrystalParameters.**calc_B_RR**(*latticeparameters*, *directspace=1*, *setvolume=False*)

- Calculate B0 matrix (columns = vectors a*,b*,c*) from direct (real) space lattice parameters (directspace=1)
- Calculate a matrix (columns = vectors a,b,c) from direct (real) space lattice parameters (directspace=0)

$\boldsymbol{q}_{ortho} = B_0\mathbf{G}^*$ where $\mathbf{G}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$

Parameters

- **latticeparameters** –
  - [a,b,c, alpha, beta, gamma] (angles are in degrees) if directspace=1
  - [a*,b*,c*, alpha*, beta*, gamma*] (angles are in degrees) if directspace=0
- **directspace** –
  - **1 (default) converts (reciprocal) direct lattice parameters** to (direct) reciprocal space calculates "B" matrix in the reciprocal space of input latticeparameters
  - **0 converts (reciprocal) direct lattice parameters to (reciprocal) direct space** calculates "B" matrix in same space of input latticeparameters
- **setvolume** –
  - False, sets direct unit cell volume to the true volume from lattice parameters
  - 1, sets direct unit cell volume to 1

- 'a**3', sets direct unit cell volume to a**3
- 'b**3', sets direct unit cell volume to b**3
- 'c**3', sets direct unit cell volume to c**3

Returns B Matrix (triangular up) from crystal (reciprocal space) frame to orthonormal frame matrix

Return type numpy array

B matrix is used in q=U B G* formula or as B0 in q= (UB) B0 G*

after Busing Levy, Acta Crysta 22 (1967), p 457

$$\begin{pmatrix} a^* & b^*\cos\gamma^* & c^*\cos beta^* \\ 0 & b^*\sin\gamma^* & -c^*\sin\beta^*\cos\alpha \\ 0 & 0 & c^*\sin\beta^*\sin\alpha \end{pmatrix}$$

with

$$\cos(\alpha) = (\cos\beta^*\cos\gamma^* - \cos\alpha^*)/(\sin\beta^*\sin\gamma^*)$$

and

$$c^*\sin\beta^*\sin\alpha = 1/c$$

LaueTools.CrystalParameters.**DeviatoricStrain_LatticeParams**(*newUBmat*, *latticeparams*, *constantlength='a'*)

Computes deviatoric strain and new direct (real) lattice parameters from matrix newUBmat (rotation and deformation) considering that one lattice length is chosen to be constant

Zero strain corresponds to reference state of input *lattice parameters*

Parameters

- **newUBmat** – (3x3) matrix operator including rotation and deformation
- **latticeparams** – 6 lattice parameters [a,b,c,:math:*alpha, beta, gamma*] in Angstrom and degrees
- **constantlength** – 'a','b', or 'c' to set one length according to the value in *latticeparams*

Returns

- 3x3 deviatoric strain tensor)
- lattice_parameter_direct_strain (direct (real) lattice parameters)

Return type 3x3 numpy array, 6 elements list

Note:

- q = newUBmat . B0 . G* where B0 (triangular up matrix) comes from lattice parameters input.
- equivalently, q = UBstar_s . G*

LaueTools.CrystalParameters.**VolumeCell**(*latticeparameters*)

Computes unit cell volume from lattice parameters (either real or reciprocal)

Parameters **latticeparameters** – 6 lattice parameters

Returns scalar volume

LaueTools.CrystalParameters.**VolumeCell**(*latticeparameters*)
Computes unit cell volume from lattice parameters (either real or reciprocal)

Parameters **latticeparameters** – 6 lattice parameters

Returns scalar volume

LaueTools.CrystalParameters.**matrix_to_rlat**(*mat*, *angles_in_deg=1*)
Returns RECIPROCAL lattice parameters of the unit cell a*,b*,c* in columns of *mat*

Parameters **mat** – matrix where columns are respectively a*,b*,c* coordinates in orthonormal frame

Returns [a*,b*,c*, alpha*, beta*, gamma*] (angles are in degrees)

Note: Reciprocal lattice parameters are contained in UB matrix : q = mat G*

7.2.2 Laue Pattern Simulation

Core module to compute Laue Pattern in various geometry

Main author is J. S. Micha: micha [at] esrf [dot] fr

version July 2019 from LaueTools package hosted in

http://sourceforge.net/projects/lauetools/

or

https://gitlab.esrf.fr/micha/lauetools

LaueTools.lauecore.**Quicklist**(*OrientMatrix*, *ReciprocBasisVectors*, *listRSnorm*, *lambdamin*, *verbose=0*)
return 6 indices min and max boundary values for each Miller index h, k, l to be contained in the largest Ewald Sphere.

Parameters

- **OrientMatrix** – orientation matrix (3*3 matrix)
- **ReciprocBasisVectors** – list of the three vectors a*,b*,c* in the lab frame before rotation with OrientMatrix
- **listRSnorm** – : list of the three reciprocal space lengthes of a*,b*,c*
- **lambdamin** – : lambdamin (in Angstrom) corresponding to energy max

Returns [[hmin,hmax],[kmin,kmax],[lmin,lmax]]

LaueTools.lauecore.**genHKL_np**(*listn*, *Extinc*)
Generate all Miller indices hkl from indices limits given by listn and taking into account for systematic exctinctions

Parameters

- **listn** (*[[hmin,hmax],[kmin,kmax],[lmin,lmax]]*) – Miller indices limits (warning: these lists are used in python range (last index is excluded))
- **Extinc** (*string*) – label corresponding to systematic exctinction rules on h k and l miller indics such as ('fcc', 'bcc', 'dia', ...) or 'no' for any rules

Returns array of [h,k,l]

Note: node [0,0,0] is excluded

LaueTools.lauecore.**getLaueSpots**(*wavelmin*, *wavelmax*, *crystalsParams*, *linestowrite*, *kf_direction='Z>0'*, *OpeningAngleCollection=22.0*, *fastcompute=0*, *ResolutionAngstrom=False*, *fileOK=1*, *verbose=1*, *dictmaterials=None*)

Compute Qxyz vectors and corresponding HKL miller indices for nodes in recicprocal space that can be measured for the given detection geometry and energy bandpass configuration.

Parameters

- **wavelmin** – smallest wavelength in Angstrom
- **wavelmax** – largest wavelength in Angstrom
- **crystalsParams** – list of *SingleCrystalParams*, each of them being a list of 4 elements for crystal orientation and strain properties:
  - **[0](array): is the B matrix a*,b*,c* vectors are expressed in column** in LaueTools frame in reciprocal angstrom units
  - [1](str): peak Extinction rules ('no','fcc','dia', etc...)
  - [2](array): orientation matrix
  - [3](str): key for material element
- **kf_direction** – string defining the average geometry, mean value of exit scattered vector: 'Z>0' top spots

  'Y>0' one side spots (towards hutch door)

  'Y<0' other side spots

  'X>0' transmission spots

  'X<0' backreflection spots
- **fastcompute** –
  - 1, compute reciprocal space (RS) vector BUT NOT the Miller indices
  - 0, returns both RS vectors (normalised) and Miller indices
- **ResolutionAngstrom** –
  - scalar, smallest interplanar distance ordered in crystal in angstrom.
  - None, all reflections will be calculated that can be time-consuming for large unit cell
- **linestowrite** – list of [string] that can be write in file or display in stdout. Example: [[""]] or [["******"],["lauetools"]]

Returns

- list of [Qx,Qy,Qz]s for each grain, list of [H,K,L]s for each grain (fastcompute = 0)
- list of [Qx,Qy,Qz]s for each grain, None (fastcompute = 1)

Caution: This method doesn't create spot instances.

This is done in filterLaueSpots with fastcompute = 0

Caution: finer selection of nodes : on camera , without harmonics can be done later with filterLaueSpots()

Note: lauetools laboratory frame is in this case: x// ki (center of ewald sphere has neagtive x component) z perp to x and belonging to the plane defined by x and dd vectors (where dd vector is the smallest vector joining sample impact point and points on CCD plane) y is perpendicular to x and z

LaueTools.lauecore.**create_spot**(*pos_vec*, *miller*, *detectordistance*, *allattributes=False*, *pixelsize=0.08056640625*, *dim=(2048*, *2048)*)

From reciprocal space position and 3 miller indices create a spot instance (on top camera geometry)

Parameters

- **pos_vec** (*list of 3 float*) – 3D vector
- **miller** – list of 3 miller indices
- **detectordistance** – approximate distance detector sample (to compute complementary spots attributes)
- **allattributes** – False or 0 not to compute complementary spot attributes
- **allattributes** – boolean

Returns spot instance

Note: spot.Qxyz is a vector expressed in lauetools frame

X along x-ray and Z towards CCD when CCD on top and y towards experimental hutch door

LaueTools.lauecore.**create_spot_np**(*Qxyz*, *miller*, *detectordistance*, *allattributes=False*, *pixelsize=0.08056640625*, *dim=(2048*, *2048)*)

From reciprocal space position and 3 miller indices create a spot instance (on top camera geometry)

Parameters

- **pos_vec** (*list of 3 float*) – 3D vector
- **miller** – list of 3 miller indices
- **detectordistance** – approximate distance detector sample (to compute complementary spots attributes)
- **allattributes** – False or 0 not to compute complementary spot attributes
- **allattributes** – boolean

Returns spot instance

Note: spot.Qxyz is a vector expressed in lauetools frame

X along x-ray and Z towards CCD when CCD on top and y towards experimental hutch door

LaueTools.lauecore.**filterLaueSpots**(*vec_and_indices, HarmonicsRemoval=1, fastcompute=0, kf_direction='Z>0', fileOK=0, detectordistance=70.0, detectordiameter=165.0, pixelsize=0.08056640625, dim=(2048, 2048), linestowrite=[['']]*)

Calculates list of grains spots on camera and without harmonics and on CCD camera from [[spots grain 0],[spots grain 1],etc] => returns [[spots grain 0],[spots grain 1],etc] w / o harmonics and on camera CCD

Parameters

- **vec_and_indices** – list of elements corresponding to 1 grain, each element is composed by * [0] array of vector
  - [1] array of indices
- **HarmonicsRemoval** – 1, removes harmonics according to their miller indices (only for fastcompute = 0)
- **fastcompute** –
  - **1, outputs a list for each grain of 2theta spots and a list for each grain of chi spots** (HARMONICS spots are still HERE!)
  - 0, outputs list for each grain of spots with
- **kf_direction** (*string*) – label for detection geometry (CCD plane with respect to the incoming beam and sample)

Returns

- list of spot instances if fastcompute=0
- 2theta, chi if fastcompute=1

Note:

- USED IMPORTANTLY in lauecore.SimulateResults lauecore.SimulateLaue
- USED in matchingrate.AngularResidues
- USED in ParametricLaueSimulator.dosimulation_parametric
- USED in AutoindexationGUI.OnSimulate_S3, DetectorCalibration.Reckon_2pts, and others

---

Todo: add dim in create_spot in various geometries

LaueTools.lauecore.**get2ThetaChi_geometry**(*oncam_vec*, *oncam_HKL*, *detectordistance=70.0*, *pixelsize=0.08056640625*, *dim=(2048, 2048)*, *kf_direction='Z>0'*)

computes list of spots instances from oncam_vec (q 3D vectors) and oncam_HKL (miller indices 3D vectors)

Parameters

- **oncam_vec** (*array with 3D elements (shape = (n,3))*) – q vectors [qx,qy,qz] (corresponding to kf collected on camera)
- **dim** (*list or tuple of 2 integers*) – CCD frame dimensions (nb pixels, nb pixels)
- **detectordistance** – approximate distance detector sample
- **detectordistance** – float or integer
- **pixelsize** (*float*) – pixel size in mm

Param kf_direction : label for detection geometry (CCD plane with respect to the incoming beam and sample)

Type kf_direction: string

Returns list of spot instances

Note: USED in lauecore.filterLaueSpots

Todo:

- to be replaced by something else not using spot class
- put this function in LaueGeometry module ?

LaueTools.lauecore.**calcSpots_fromHKLlist**(*UB*, *B0*, *HKL*, *dictCCD*)

computes all Laue Spots properties on 2D detector from a list of hkl (given structure by B0 matrix, orientation by UB matrix, and detector geometry by dictCCD)

Parameters

- **UB** (*3x3 array (or list)*) – orientation matrix (rotation -and if any- strain)
- **B0** (*3x3 array (or list)*) – initial a*,b*,c* reciprocal unit cell basis vector in Laue-tools frame (x// ki))
- **HKL** (*array with shape = (n, 3)*) – array of Miller indices
- **dictCCD** – dictionnary of CCD properties (with key 'CCDparam', 'pixelsize','dim') for 'ccdparam' 5 CCD calibration parameters [dd,xcen,ycen,xbet,xgam], pixelsize in mm, and (dim1, dim2)
- **dictCCD** – dict object

Returns list of arrays H, K, L, Qx, Qy, Qz, X, Y, twthe, chi, Energy

Fundamental equation $\mathbf{q} = UB * B0 * \mathbf{G}^*$ with $\mathbf{G}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$

Note: USED in DetectorCalibration.OnWriteResults, and PlotRefineGUI.onWriteFitFile

LaueTools.lauecore.**SimulateLaue**(*grain, emin, emax, detectorparameters, kf_direction='Z>0', ResolutionAngstrom=False, removeharmonics=0, pixelsize=0.08056640625, dim=(2048, 2048), detectordiameter=None, force_extinction=None, dictmaterials={'Al': ['Al', [4.05, 4.05, 4.05, 90, 90, 90], 'fcc'], 'Al2Cu': ['Al2Cu', [6.063, 6.063, 4.872, 90, 90, 90], 'no'], 'Al2O3': ['Al2O3', [4.785, 4.785, 12.991, 90, 90, 120], 'Al2O3'], 'Al2O3_all': ['Al2O3_all', [4.785, 4.785, 12.991, 90, 90, 120], 'no'], 'AlN': ['AlN', [3.11, 3.11, 4.98, 90.0, 90.0, 120.0], 'wurtzite'], 'Au': ['Au', [4.078, 4.078, 4.078, 90, 90, 90], 'fcc'], 'CCDL1949': ['CCDL1949', [9.89, 17.85, 5.31, 90, 107.5, 90], 'h+k=2n'], 'CdHgTe': ['CdHgTe', [6.46678, 6.46678, 6.46678, 90, 90, 90], 'dia'], 'CdHgTe_fcc': ['CdHgTe_fcc', [6.46678, 6.46678, 6.46678, 90, 90, 90], 'fcc'], 'CdTe': ['CdTe', [6.487, 6.487, 6.487, 90, 90, 90], 'fcc'], 'CdTeDiagB': ['CdTeDiagB', [4.5721, 7.9191, 11.1993, 90, 90, 90], 'no'], 'Crocidolite': ['Crocidolite', [9.811, 18.013, 5.326, 90, 103.68, 90], 'no'], 'Crocidolite_2': ['Crocidolite_2', [9.76, 17.93, 5.35, 90, 103.6, 90], 'no'], 'Crocidolite_2_72deg': ['Crocidolite_2', [9.76, 17.93, 5.35, 90, 76.4, 90], 'no'], 'Crocidolite_small': ['Crocidolite_small', [3.2533333333333334, 5.976666666666667, 1.7833333333333332, 90, 103.6, 90], 'no'], 'Crocidolite_whittaker_1949': ['Crocidolite_whittaker_1949', [9.89, 17.85, 5.31, 90, 107.5, 90], 'no'], 'Cu': ['Cu', [3.6, 3.6, 3.6, 90, 90, 90], 'fcc'], 'Cu6Sn5_monoclinic': ['Cu6Sn5_monoclinic', [11.02, 7.28, 9.827, 90, 98.84, 90], 'no'], 'Cu6Sn5_tetra': ['Cu6Sn5_tetra', [3.608, 3.608, 5.037, 90, 90, 90], 'no'], 'DIA': ['DIA', [5.0, 5.0, 5.0, 90, 90, 90], 'dia'], 'DIAs': ['DIAs', [3.56683, 3.56683, 3.56683, 90, 90, 90], 'dia'], 'DarinaMolecule': ['DarinaMolecule', [9.4254, 13.5004, 13.8241, 61.83, 84.555, 75.231], 'no'], 'FCC': ['FCC', [5.0, 5.0, 5.0, 90, 90, 90], 'fcc'], 'Fe': ['Fe', [2.856, 2.856, 2.856, 90, 90, 90], 'bcc'], 'Fe2Ta': ['Fe2Ta', [4.83, 4.83, 0.788, 90, 90, 120], 'no'], 'FeAl': ['FeAl', [5.871, 5.871, 5.871, 90, 90, 90], 'fcc'], 'GaAs': ['GaAs', [5.65325, 5.65325, 5.65325, 90, 90, 90], 'dia'], 'GaN': ['GaN', [3.189, 3.189, 5.185, 90, 90, 120], 'wurtzite'], 'GaN_all': ['GaN_all', [3.189, 3.189, 5.185, 90, 90, 120], 'no'], 'Ge': ['Ge', [5.6575, 5.6575, 5.6575, 90, 90, 90], 'dia'], 'Ge_compressedhydro': ['Ge_compressedhydro', [5.64, 5.64, 5.64, 90, 90, 90.0], 'dia'], 'Ge_s': ['Ge_s', [5.6575, 5.6575, 5.6575, 90, 90, 89.5], 'dia'], 'Getest': ['Getest', [5.6575, 5.6575, 5.6574, 90, 90, 90], 'dia'], 'Hematite': ['Hematite', [5.03459, 5.03459, 13.7533, 90, 90, 120], 'no'], 'In': ['In', [3.2517, 3.2517, 4.9459, 90, 90, 90], 'h+k+l=2n'], 'InGaN': ['InGaN', [3.3609999999999998, 3.3609999999999998, 5.439, 90, 90, 120], 'wurtzite'], 'InN': ['InN', [3.533, 3.533, 5.693, 90, 90, 120], 'wurtzite'], 'Magnetite': ['Magnetite', [8.391, 8.391, 8.391, 90, 90, 90], 'dia'], 'Magnetite_fcc': ['Magnetite_fcc', [8.391, 8.391, 8.391, 90, 90, 90], 'fcc'], 'Magnetite_sc': ['Magnetite_sc', [8.391, 8.391, 8.391, 90, 90, 90], 'no'], 'Nd45': ['Nd45', [5.4884, 5.4884, 5.4884, 90, 90, 90], 'fcc'], 'Ni': ['Ni', [3.5238, 3.5238, 3.5238, 90, 90, 90], 'fcc'], 'NiO': ['NiO', [2.96, 2.96, 7.23, 90, 90, 120], 'no'], 'NiTi': ['NiTi', [3.5506, 3.5506, 3.5506, 90, 90, 90], 'fcc'], 'SC': ['SC', [1.0, 1.0, 1.0, 90, 90, 90], 'no'], 'SC5': ['SC5', [5.0, 5.0, 5.0, 90, 90, 90], 'no'], 'SC7': ['SC7', [7.0, 7.0, 7.0, 90, 90, 90], 'no'], 'Si': ['Si', [5.4309, 5.4309, 5.4309, 90, 90, 90], 'dia'], 'Sn': ['Sn', [5.83, 5.83, 3.18, 90, 90, 90], 'h+k+l=2n'], 'Ti': ['Ti', [2.95, 2.95, 4.68, 90,*

Computes Laue Pattern spots positions, scattering angles, miller indices for a SINGLE grain or Xtal

Parameters

- **grain** – crystal parameters made of a 4 elements list
- **emin** – minimum bandpass energy (keV)
- **emax** – maximum bandpass energy (keV)
- **removeharmonics** –
  - **1, removes harmonics spots and keep fondamental spots (or reciprocal direction)** (with lowest Miller indices)
  - 0 keep all spots (including harmonics)

Returns single grain data: Twicetheta, Chi, Miller_ind, posx, posy, Energy

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Todo: To update to accept kf_direction not only in reflection geometry

---

Note: USED in detectorCalibration. . . simulate_theo for non routine geometry (ie except Z>0 (reflection top) X>0 (transmission)

LaueTools.lauecore.**SimulateLaue_full_np**(*grain, emin, emax, detectorparameters, kf_direction='Z>0', ResolutionAngstrom=False, removeharmonics=0, pixelsize=0.08056640625, dim=(2048, 2048), detectordiameter=None, force_extinction=None, dictmaterials={'Al': ['Al', [4.05, 4.05, 4.05, 90, 90, 90], 'fcc'], 'Al2Cu': ['Al2Cu', [6.063, 6.063, 4.872, 90, 90, 90], 'no'], 'Al2O3': ['Al2O3', [4.785, 4.785, 12.991, 90, 90, 120], 'Al2O3'], 'Al2O3_all': ['Al2O3_all', [4.785, 4.785, 12.991, 90, 90, 120], 'no'], 'AlN': ['AlN', [3.11, 3.11, 4.98, 90.0, 90.0, 120.0], 'wurtzite'], 'Au': ['Au', [4.078, 4.078, 4.078, 90, 90, 90], 'fcc'], 'CCDL1949': ['CCDL1949', [9.89, 17.85, 5.31, 90, 107.5, 90], 'h+k=2n'], 'CdHgTe': ['CdHgTe', [6.46678, 6.46678, 6.46678, 90, 90, 90], 'dia'], 'CdHgTe_fcc': ['CdHgTe_fcc', [6.46678, 6.46678, 6.46678, 90, 90, 90], 'fcc'], 'CdTe': ['CdTe', [6.487, 6.487, 6.487, 90, 90, 90], 'fcc'], 'CdTeDiagB': ['CdTeDiagB', [4.5721, 7.9191, 11.1993, 90, 90, 90], 'no'], 'Crocidolite': ['Crocidolite', [9.811, 18.013, 5.326, 90, 103.68, 90], 'no'], 'Crocidolite_2': ['Crocidolite_2', [9.76, 17.93, 5.35, 90, 103.6, 90], 'no'], 'Crocidolite_2_72deg': ['Crocidolite_2', [9.76, 17.93, 5.35, 90, 76.4, 90], 'no'], 'Crocidolite_small': ['Crocidolite_small', [3.2533333333333334, 5.976666666666667, 1.7833333333333332, 90, 103.6, 90], 'no'], 'Crocidolite_whittaker_1949': ['Crocidolite_whittaker_1949', [9.89, 17.85, 5.31, 90, 107.5, 90], 'no'], 'Cu': ['Cu', [3.6, 3.6, 3.6, 90, 90, 90], 'fcc'], 'Cu6Sn5_monoclinic': ['Cu6Sn5_monoclinic', [11.02, 7.28, 9.827, 90, 98.84, 90], 'no'], 'Cu6Sn5_tetra': ['Cu6Sn5_tetra', [3.608, 3.608, 5.037, 90, 90, 90], 'no'], 'DIA': ['DIA', [5.0, 5.0, 5.0, 90, 90, 90], 'dia'], 'DIAs': ['DIAs', [3.56683, 3.56683, 3.56683, 90, 90, 90], 'dia'], 'DarinaMolecule': ['DarinaMolecule', [9.4254, 13.5004, 13.8241, 61.83, 84.555, 75.231], 'no'], 'FCC': ['FCC', [5.0, 5.0, 5.0, 90, 90, 90], 'fcc'], 'Fe': ['Fe', [2.856, 2.856, 2.856, 90, 90, 90], 'bcc'], 'Fe2Ta': ['Fe2Ta', [4.83, 4.83, 0.788, 90, 90, 120], 'no'], 'FeAl': ['FeAl', [5.871, 5.871, 5.871, 90, 90, 90], 'fcc'], 'GaAs': ['GaAs', [5.65325, 5.65325, 5.65325, 90, 90, 90], 'dia'], 'GaN': ['GaN', [3.189, 3.189, 5.185, 90, 90, 120], 'wurtzite'], 'GaN_all': ['GaN_all', [3.189, 3.189, 5.185, 90, 90, 120], 'no'], 'Ge': ['Ge', [5.6575, 5.6575, 5.6575, 90, 90, 90], 'dia'], 'Ge_compressedhydro': ['Ge_compressedhydro', [5.64, 5.64, 5.64, 90, 90, 90.0], 'dia'], 'Ge_s': ['Ge_s', [5.6575, 5.6575, 5.6575, 90, 90, 89.5], 'dia'], 'Getest': ['Getest', [5.6575, 5.6575, 5.6574, 90, 90, 90], 'dia'], 'Hematite': ['Hematite', [5.03459, 5.03459, 13.7533, 90, 90, 120], 'no'], 'In': ['In', [3.2517, 3.2517, 4.9459, 90, 90, 90], 'h+k+l=2n'], 'InGaN': ['InGaN', [3.3609999999999998, 3.3609999999999998, 5.439, 90, 90, 120], 'wurtzite'], 'InN': ['InN', [3.533, 3.533, 5.693, 90, 90, 120], 'wurtzite'], 'Magnetite': ['Mag-*

Compute Laue Pattern spots positions, scattering angles, miller indices for a SINGLE grain or Xtal using numpy vectorization

Parameters

- **grain** – crystal parameters in a 4 elements list
- **emin** – minimum bandpass energy (keV)
- **emax** – maximum bandpass energy (keV)
- **removeharmonics** – 1, remove harmonics spots and keep fondamental spots (with lowest Miller indices)

Returns single grain data: Twicetheta, Chi, Miller_ind, posx, posy, Energy

---

Todo: update to accept kf_direction not only in reflection geometry

---

Note: USED in detectorCalibration... simulate_theo for routine geometry Z>0 (reflection top) X>0 (transmission)

LaueTools.lauecore.**SimulateResult**(*grain, emin, emax, simulparameters, fastcompute=1, ResolutionAngstrom=False, dictmaterials={'Al': ['Al', [4.05, 4.05, 4.05, 90, 90, 90], 'fcc'], 'Al2Cu': ['Al2Cu', [6.063, 6.063, 4.872, 90, 90, 90], 'no'], 'Al2O3': ['Al2O3', [4.785, 4.785, 12.991, 90, 90, 120], 'Al2O3'], 'Al2O3_all': ['Al2O3_all', [4.785, 4.785, 12.991, 90, 90, 120], 'no'], 'AlN': ['AlN', [3.11, 3.11, 4.98, 90.0, 90.0, 120.0], 'wurtzite'], 'Au': ['Au', [4.078, 4.078, 4.078, 90, 90, 90], 'fcc'], 'CCDL1949': ['CCDL1949', [9.89, 17.85, 5.31, 90, 107.5, 90], 'h+k=2n'], 'CdHgTe': ['CdHgTe', [6.46678, 6.46678, 6.46678, 90, 90, 90], 'dia'], 'CdHgTe_fcc': ['CdHgTe_fcc', [6.46678, 6.46678, 6.46678, 90, 90, 90], 'fcc'], 'CdTe': ['CdTe', [6.487, 6.487, 6.487, 90, 90, 90], 'fcc'], 'CdTeDiagB': ['CdTeDiagB', [4.5721, 7.9191, 11.1993, 90, 90, 90], 'no'], 'Crocidolite': ['Crocidolite', [9.811, 18.013, 5.326, 90, 103.68, 90], 'no'], 'Crocidolite_2': ['Crocidolite_2', [9.76, 17.93, 5.35, 90, 103.6, 90], 'no'], 'Crocidolite_2_72deg': ['Crocidolite_2', [9.76, 17.93, 5.35, 90, 76.4, 90], 'no'], 'Crocidolite_small': ['Crocidolite_small', [3.2533333333333334, 5.976666666666667, 1.7833333333333332, 90, 103.6, 90], 'no'], 'Crocidolite_whittaker_1949': ['Crocidolite_whittaker_1949', [9.89, 17.85, 5.31, 90, 107.5, 90], 'no'], 'Cu': ['Cu', [3.6, 3.6, 3.6, 90, 90, 90], 'fcc'], 'Cu6Sn5_monoclinic': ['Cu6Sn5_monoclinic', [11.02, 7.28, 9.827, 90, 98.84, 90], 'no'], 'Cu6Sn5_tetra': ['Cu6Sn5_tetra', [3.608, 3.608, 5.037, 90, 90, 90], 'no'], 'DIA': ['DIA', [5.0, 5.0, 5.0, 90, 90, 90], 'dia'], 'DIAs': ['DIAs', [3.56683, 3.56683, 3.56683, 90, 90, 90], 'dia'], 'DarinaMolecule': ['DarinaMolecule', [9.4254, 13.5004, 13.8241, 61.83, 84.555, 75.231], 'no'], 'FCC': ['FCC', [5.0, 5.0, 5.0, 90, 90, 90], 'fcc'], 'Fe': ['Fe', [2.856, 2.856, 2.856, 90, 90, 90], 'bcc'], 'Fe2Ta': ['Fe2Ta', [4.83, 4.83, 0.788, 90, 90, 120], 'no'], 'FeAl': ['FeAl', [5.871, 5.871, 5.871, 90, 90, 90], 'fcc'], 'GaAs': ['GaAs', [5.65325, 5.65325, 5.65325, 90, 90, 90], 'dia'], 'GaN': ['GaN', [3.189, 3.189, 5.185, 90, 90, 120], 'wurtzite'], 'GaN_all': ['GaN_all', [3.189, 3.189, 5.185, 90, 90, 120], 'no'], 'Ge': ['Ge', [5.6575, 5.6575, 5.6575, 90, 90, 90], 'dia'], 'Ge_compressedhydro': ['Ge_compressedhydro', [5.64, 5.64, 5.64, 90, 90, 90.0], 'dia'], 'Ge_s': ['Ge_s', [5.6575, 5.6575, 5.6575, 90, 90, 89.5], 'dia'], 'Getest': ['Getest', [5.6575, 5.6575, 5.6574, 90, 90, 90], 'dia'], 'Hematite': ['Hematite', [5.03459, 5.03459, 13.7533, 90, 90, 120], 'no'], 'In': ['In', [3.2517, 3.2517, 4.9459, 90, 90, 90], 'h+k+l=2n'], 'InGaN': ['InGaN', [3.3609999999999998, 3.3609999999999998, 5.439, 90, 90, 120], 'wurtzite'], 'InN': ['InN', [3.533, 3.533, 5.693, 90, 90, 120], 'wurtzite'], 'Magnetite': ['Magnetite', [8.391, 8.391, 8.391, 90, 90, 90], 'dia'], 'Magnetite_fcc': ['Magnetite_fcc', [8.391, 8.391, 8.391, 90, 90, 90], 'fcc'], 'Magnetite_sc': ['Magnetite_sc', [8.391, 8.391, 8.391, 90, 90, 90], 'no'], 'Nd45': ['Nd45', [5.4884, 5.4884, 5.4884, 90, 90, 90], 'fcc'], 'Ni': ['Ni', [3.5238, 3.5238, 3.5238, 90, 90, 90], 'fcc'], 'NiO': ['NiO', [2.96, 2.96, 7.23, 90, 90, 120], 'no'], 'NiTi': ['NiTi', [3.5506, 3.5506, 3.5506, 90, 90, 90], 'fcc'], 'SC': ['SC', [1.0, 1.0, 1.0, 90, 90, 90], 'no'], 'SC5': ['SC5', [5.0, 5.0, 5.0, 90, 90, 90], 'no'], 'SC7': ['SC7', [7.0, 7.0, 7.0, 90, 90, 90], 'no'], 'Sb': ['Sb', [4.3, 4.3, 11.3, 90, 90, 120], 'no'], 'Si': ['Si', [5.4309, 5.4309, 5.4309, 90, 90, 90], 'dia'], 'Sn': ['Sn', [5.83, 5.83, 3.18,*

Simulates 2theta chi of Laue Pattern spots for ONE SINGLE grain

Parameters

- **grain** – crystal parameters in a 4 elements list
- **emin** – minimum bandpass energy (keV)
- **emax** – maximum bandpass energy (keV)

Returns 2theta, chi

Warning: Need of approximate detector distance and diameter to restrict simulation to a limited solid angle

Note:

- USED: in AutoindexationGUI.OnStart, LaueToolsGUI.OnCheckOrientationMatrix
- USED also IndexingImageMatching, lauecore.SimulateLaue_merge

7.2.3 2D Detection Geometry

Module of lauetools project to compute Laue spots position on CCD camera. It handles detection and source geometry.

Warning: The frame (LT2) considered in this package (with y axis parallel to the incoming beam) in not the LaueTools frame (for which x is parallel to the incoming beam)

JS Micha June 2019

- **Vectors Definitions**
  - **q** momentum transfer vector from resp. incoming and outgoing wave vector **ki** and **kf**, $q = kf - ki$
  - When a Laue spot exists, **q** is equal to the one node of the reciprocal lattice given by **G*** vector
  - **G* is perpendicular to atomic planes defined by the three Miller indices h,k,l** such as **G***=h**a*** + k**b*** +l**c*** where **a***, **b***, and **c*** are the unit cell lattice basis vectors.
  - **kf**: scattered beam vector whose corresponding unit vector is **uf**
  - **ki** incoming beam vector, **ui** corresponding unit vector
- **Laboratory Frame LT2**
  - I: origin
  - z vertical up perpendicular to CCD plane (top camera geometry)
  - y along X-ray horizontal
  - x towards wall behind horizontal
  - O: origin of pixel CCD frame in detecting plane
  - **j // ui** incoming beam unit vector
  - **z axis is defined by the CCD camera position. z axis is perpendicular to CCD plane** such as IO belongs to the plane Iyz

- bet: angle between **IO** and **k**
- **i**= **j**^**k (when entering the BM32 hutch i is approximately towards the wall** (in CCD on top geometry and beam coming from the right)
- M: point lying in CCD plane corresponding to Laue spot
- **uf** is the unit vector relative to vector **IM**

kf is also a vector collinear to **IM** with a length of R=1/wavelength=E/12.398 [keV] with wavelength and Energy of the corresponding bragg's reflections.

I is the point from which calibration parameters (CCD position) are deduced (from a perfectly known crystal structure Laue pattern) Iprime is an other source of emission (posI or offset in functions)

2θ is the scattering angle between **ui** and **uf**, i.e.

$\cos(2\theta) = u_i.u_f$

$$\mathbf{k_f} = (-\sin 2\theta \sin\chi, \cos 2\theta, \sin 2\theta \cos\chi)$$
$$\mathbf{k_i} = (0, 1, 0)$$

Energy= 12.398* q**2/(2* **q**.**ui**)=12.398 * q**2/ (-2 sin theta)

Calibration parameters (CCD position and detection geometry)

- calib: list of the 5 calibration parameters [dd,xcen,ycen,xbet,xgam]
- dd: norm of **IO** [mm]
- **xcen,ycen [pixel unit]: pixels values in CCD frame of point O with respect to Oprime where** Oprime is the origin of CCD pixels frame (at a corner of the CCD array)
- xbet: angle between **IO** and **k** [degree]
- **xgam: azimutal rotation angle around z axis. Angle between CCD array axes** and (**i**,**j**) after rotation by xbet [degree].

sample frame

Origin is I and unit frame vectors (**is**, **js**, **ks**) are derived from absolute frame by the rotation (axis= - **i**, angle= wo) where wo is the angle between **js** and **j**

`LaueTools.LaueGeometry.`**`calc_uflab`**(*xcam*, *ycam*, *detectorplaneparameters*, *offset=0*, *returnAngles=1*, *verbose=0*, *pixelsize=0.08056640625*, *rectpix=0*, *kf_direction='Z>0'*)

Computes unit vector $\mathbf{u_f} = \frac{\mathbf{k_f}}{\|k_f\|}$ in laboratory frame of scattered beam k_f (angle scattering angles 2theta and chi) from X, Y pixel Laue spot position

Unit vector uf correspond to normalized kf vector: q = kf - ki from lists of X and Y Laue spots pixels positions on detector

Parameters

- **`xcam`** (*`list of floats`*) – list of pixel X position
- **`ycam`** (*`list of floats`*) – list of pixel Y position
- **`detectorplaneparameters`** – list of 5 calibration parameters
- **`offset`** – float, offset in position along incoming beam of source of scattered rays if positive: offset in sample depth units: mm

Returns

- if returnAngles=1 : twicetheta, chi *(default)*

- if returnAngles!=1 : uflab, IMlab

LaueTools.LaueGeometry.**calc_uflab_trans**(*xcam*, *ycam*, *calib*, *returnAngles=1*, *verbose=0*, *pixelsize=0.08056640625*, *rectpix=0*)

compute 2θ and χ scattering angles or **uf** and **kf** vectors from lists of X and Y Laue spots positions in TRANSMISSION geometry

Parameters

- **xcam** (*list of floats*) – list of pixel X position
- **ycam** (*list of floats*) – list of pixel Y position
- **calib** – list of 5 calibration parameters

Returns

- if returnAngles=1 : twicetheta, chi *(default)*
- if returnAngles!=1 : uflab, IMlab

TODO: add offset like in reflection geometry

LaueTools.LaueGeometry.**calc_xycam**(*uflab*, *calib*, *energy=0*, *offset=None*, *verbose=0*, *returnIpM=False*, *pixelsize=0.08056640625*, *dim=(2048, 2048)*, *rectpix=0*)

Computes Laue spots position x and y in pixels units in CCD frame from unit scattered vector uf expressed in Lab. frame

computes coordinates of point M on CCD from point source and **uflab**. Point Ip (source Iprime of x-ray scattered beams) (for each Laue spot **uflab** is the unit vector of **IpM**) Point Ip is shifted by offset (if not None) from the default point I (used to calibrate the CCD camera and 2theta chi determination)

th0 (theta in degrees) Energy (energy in keV)

Parameters

- **uflab** (*list or array (length must > 1)*) – list or array of [qx,qy,qz] (q vector)
- **calib** (*list of floats*) – list 5 detector calibration parameters
- **offset** (*list of floats ([x,y,z])*) – offset (in mm) in the scattering source (origin of Laue spots) position with respect to the position which has been used for the calibration of the CCD detector plane. Offset is positive when in the same direction as incident beam (i.e. in sample depth) (incident beam direction remains constant)

Returns

- xcam: list of pixel X coordinates
- ycam: list of pixel Y coordinates
- theta: list half scattering angle "theta" (in degree)
- optionally energy=1: add in output list of spot energies (in keV)
- if returnIpM and offset not None: return list of vectors **IprimeM**

LaueTools.LaueGeometry.**calc_xycam_transmission**(*uflab*, *calib*, *energy=0*, *offset=None*, *verbose=0*, *returnIpM=False*, *pixelsize=0.08056640625*, *dim=(2048, 2048)*, *rectpix=0*)

Computes Laue spots position x and y in pixels units (in CCD frame) from scattering vector q

As calc_xycam() but in TRANSMISSION geometry

LaueTools.LaueGeometry.**uflab_from2thetachi**(*twicetheta*, *chi*, *verbose=0*)

Computes $\mathbf{u_f}$ vectors coordinates in lauetools LT2 frame from $\mathbf{k_f}$ scattering angles 2θ and 2χ angles

Parameters

- **twicetheta** – (list) 2θ angle(s) (in degree)
- **chi** – (list) 2χ angle(s) (in degree)

Returns list of *{bf u_f}* = $[uf_x, uf_y, uf_z]$

Return type list

LaueTools.LaueGeometry.**from_twchi_to_qunit**(*Angles*)

from kf 2theta, chi to q unit in LaueTools frame (xx// ki) q=kf-ki returns array = (all x's, all y's, all z's)

Angles in degrees !! Angles[0] 2theta deg values, Angles[1] chi values in deg

this is the inverse function of from_qunit_to_twchi(), useful to check it

LaueTools.LaueGeometry.**from_twchi_to_q**(*Angles*)

From kf 2theta,chi to q (arbitrary lenght) in lab frame (xx// ki) q=kf-ki returns array = (all qx's, all qy's, all qz's)

Angles in degrees !! Angles[0] 2theta deg values, Angles[1] chi values in deg

LaueTools.LaueGeometry.**from_qunit_to_twchi**(*arrayXYZ*, *labXMAS=0*)

Returns 2theta chi from a q unit vector (defining a direction) expressed in LaueTools frame (**xx// ki**) **q=kf-ki**

$$\begin{bmatrix} -\sin\theta \\ \cos\theta\sin\chi \\ \cos\theta\cos\chi \end{bmatrix}$$

Note: in LaueTools frame

$$kf = \begin{bmatrix} \cos 2\theta \\ \sin 2\theta \sin\chi \\ \sin 2\theta \cos\chi \end{bmatrix}$$

$$q = 2\sin\theta \begin{bmatrix} -\sin\theta \\ \cos\theta\sin\chi \\ \cos\theta\cos\chi \end{bmatrix}$$

In LT2 Frame labXMAS=1

$$kf = \begin{bmatrix} \sin 2\theta \sin\chi \\ \cos 2\theta \\ \sin 2\theta \cos\chi \end{bmatrix}$$

$$q = 2\sin\theta \begin{bmatrix} \cos\theta\sin\chi \\ -\sin\theta \\ \cos\theta\cos\chi \end{bmatrix}$$

LaueTools.LaueGeometry.**qvector_from_xy_E**(*xcamList*, *ycamList*, *energy*, *detectorplaneparameters*, *pixelsize*)

Returns q vectors in Lauetools frame given x and y pixel positions on detector for a given Energy (keV)

Parameters

- **xcamList** – list pixel x postions
- **ycamList** – list pixel y postions
- **energy** – list pf energies

- **detectorplaneparameters** – list of 5 calibration parameters
- **pixelsize** – pixel size in mm

LaueTools.LaueGeometry.**unit_q**(*ttheta*, *chi*, *frame='lauetools'*, *anglesample=40.0*)

Returns unit q vector from 2theta,chi coordinates

Parameters

- **ttheta** – list of 2theta angles (in degrees)
- **chi** – list of chi angles (in degrees)
- **anglesample** – incidence angle of beam to surface plane (degrees)
- **frame** – frame to express vectors in: 'lauetools' , 'XMASlab' (LT2 frame),'XMASsample'

Returns list of 3D u_f (unit vector of scattering transfer q)

LaueTools.LaueGeometry.**Compute_data2thetachi**(*filename*, *tuple_column_X_Y_I*, *_nblines_headertoskip*, *sorting_intensity='yes'*, *param=None*, *kf_direction='Z>0'*, *verbose=1*, *pixelsize=0.08056640625*, *dim=(2048, 2048)*, *saturation=0*, *forceextension_lines_to_extract=None*, *col_isbadspot=None*, *alpha_xray_incidence_correction=None*)

Converts spot positions x,y to scattering angles 2theta, chi from a list of peaks

Parameters

- **filename** (*string*) – fullpath to peaks list ASCII file
- **tuple_column_X_Y_I** (*3 elements*) – tuple with column indices of spots X, Y (pixels on CCD) and intensity
- **_nblines_headertoskip** – nb of line to skip before reading an array of data in ascii file
- **param** – list of CCD calibration parameters [det, xcen, ycen, xbet, xgam]
- **pixelsize** – pixelsize in mm
- **dim** – (nb pixels x, nb pixels y)
- **kf_direction** (*string*) – label of detection geometry (CCD position): 'Z>0','X>0',...
- **sorting_intensity** – 'yes' sort spots list by decreasing intensity

saturation = 0 : do not read Ipixmax column of DAT file from LaueTools peaksearch saturation > 0 : read Ipixmax column and create data_sat list data_sat[i] = 1 if Ipixmax[i]> saturation, =0 otherwise

Note: _nblines_headertoskip =0 for .pik file (no header at all) _nblines_headertoskip =1 for .peaks coming from fit2d

col_Ipixmax = 10 for .dat from LT peak search using method "Local Maxima" (TODO : bug in Ipixmax for method "convolve")

LaueTools.LaueGeometry.**convert2corfile**(*filename*, *calibparam*, *dirname_in=None*, *dirname_out=None*, *pixelsize=0.08056640625*, *CCDCalibdict=None*, *add_props=False*)

Convert .dat (peaks list from peaksearch procedure) to .cor (adding scattering angles 2theta chi)

From X,Y pixel positions in peak list file (x,y,I,...) and detector plane geometry comptues scattering angles 2theta chi and creates a .cor file (ascii peaks list (2theta chi X Y int ...))

Parameters

- **calibparam** – list of 5 CCD cakibration parameters (used if CCDCalibdict is None or CCDCalibdict['CCDCalibPameters'] is missing)
- **pixelsize** – CCD pixelsize (in mm) (used if CCDCalibdict is None or CCDCalibdict['pixelsize'] is missing)
- **CCDCalibdict** – dictionary of CCD file and calibration parameters
- **add_props** – add all peaks properties to .cor file instead of the 5 columns

LaueTools.LaueGeometry.**convert2corfile_fileseries**(*fileindexrange*, *filenameprefix*, *calibparam*, *suffix=''*, *nbdigits=4*, *dirname_in=None*, *dirname_out=None*, *pixelsize=0.08056640625*, *fliprot='no'*)

convert a serie of peaks list ascii files to .cor files (adding scattering angles).

Filename is decomposed as following for incrementing file index in ####: prefix####suffix example: myimage_0025.myccd => prefix=myimage_ nbdigits=4 suffix=.myccd

Parameters

- **nbdigits** – nb of digits of file index in filename (with zero padding) (example: for myimage_0002.ccd nbdigits = 4
- **calibparam** – list of 5 CCD cakibration parameters

LaueTools.LaueGeometry.**convert2corfile_multiprocessing**(*fileindexrange*, *filenameprefix*, *calibparam*, *dirname_in=None*, *suffix=''*, *nbdigits=4*, *dirname_out=None*, *pixelsize=0.08056640625*, *fliprot='no'*, *nb_of_cpu=6*)

launch several processes in parallel to convert .dat file to .cor file

LaueTools.LaueGeometry.**vec_normalTosurface**(*mat_labframe*)

solve Mat * X = (0,0,1) for X for pure rotation invMat = transpose(Mat)

TODO: add option sample angle and axis

LaueTools.LaueGeometry.**vec_onsurface_alongys**(*mat_labframe*)

solve Mat * X = (0,1,0) for X for pure rotation invMat = transpose(Mat)

LaueTools.LaueGeometry.**convert_xycam_from_sourceshift**(*OMs*, *IIp*, *calib*, *verbose=0*)

From x,y on CCD camera (OMs) and source shift (IIprime) compute modified x,y values for the SAME calibration (calib)(for further analysis)

return new value of x,y

LaueTools.LaueGeometry.**lengthInSample**(*depth*, *twtheta*, *chi*, *omega*, *verbose=False*)

compute geometrical lengthes in sample from impact point (I) at the surface to a point (B) where xray are scattered (or fluorescence is emitted) and finally escape from inside at point (C) lying at the sample surface (intersection of line with unit vector u with sample surface plane tilted by omega)

Warning: twtheta and chi angles can be misleading. Assumption is made that angles of unit vector from B to C (or to detector frame pixel) are 2θ and χ. For large depth D, unit vector scattered beam direction is not given by 2θ and χ angles as they are used for describing the scattering direction from point I and a given detector frame position (you should then compute the two angles correction , actually χ is unchanged, and the 2θ change is approx d/ distance .i.e. 3 10-4 for d=20 µm and CCD at 70 mm)

Note:

incoming beam coming from the right positive x direction with

- IB = (-D,0,0)
- BC =(xc+D,yc,zc)
- and length BC is proportional to the depth D

7.2.4 Multiple Grains and Strain/orientation Distribution

Module to compute Laue Patterns from several crystals in various geometry

Main author is J. S. Micha: micha [at] esrf [dot] fr

version July 2019 from LaueTools package for python2 hosted in

http://sourceforge.net/projects/lauetools/

or for python3 and 2 in

https://gitlab.esrf.fr/micha/lauetools

`LaueTools.multigrainsSimulator.`**`Read_GrainListparameter`**(*param*)
Read dictionary of input key parameters for simulation

`LaueTools.multigrainsSimulator.`**`Construct_GrainsParameters_parametric`**(*SelectGrains_parametric*)
return list of simulation parameters for each grain set (mother and children grains)

LaueTools.multigrainsSimulator.**dosimulation_parametric**(*_list_param, Transform_params=None, SelectGrains=None, emax=25.0, emin=5.0, detectordistance=68.7, detectordiameter=165.0, posCEN=(1024.0, 1024.0), cameraAngles=(0.0, 0.0), gauge=None, kf_direction='Z>0', pixelsize=0.08056640625, framedim=(2048, 2048), dictmaterials={'Al': ['Al', [4.05, 4.05, 4.05, 90, 90, 90], 'fcc'], 'Al2Cu': ['Al2Cu', [6.063, 6.063, 4.872, 90, 90, 90], 'no'], 'Al2O3': ['Al2O3', [4.785, 4.785, 12.991, 90, 90, 120], 'Al2O3'], 'Al2O3_all': ['Al2O3_all', [4.785, 4.785, 12.991, 90, 90, 120], 'no'], 'AlN': ['AlN', [3.11, 3.11, 4.98, 90.0, 90.0, 120.0], 'wurtzite'], 'Au': ['Au', [4.078, 4.078, 4.078, 90, 90, 90], 'fcc'], 'CCDL1949': ['CCDL1949', [9.89, 17.85, 5.31, 90, 107.5, 90], 'h+k=2n'], 'CdHgTe': ['CdHgTe', [6.46678, 6.46678, 6.46678, 90, 90, 90], 'dia'], 'CdHgTe_fcc': ['CdHgTe_fcc', [6.46678, 6.46678, 6.46678, 90, 90, 90], 'fcc'], 'CdTe': ['CdTe', [6.487, 6.487, 6.487, 90, 90, 90], 'fcc'], 'CdTeDiagB': ['CdTeDiagB', [4.5721, 7.9191, 11.1993, 90, 90, 90], 'no'], 'Crocidolite': ['Crocidolite', [9.811, 18.013, 5.326, 90, 103.68, 90], 'no'], 'Crocidolite_2': ['Crocidolite_2', [9.76, 17.93, 5.35, 90, 103.6, 90], 'no'], 'Crocidolite_2_72deg': ['Crocidolite_2', [9.76, 17.93, 5.35, 90, 76.4, 90], 'no'], 'Crocidolite_small': ['Crocidolite_small', [3.2533333333333334, 5.976666666666667, 1.7833333333333332, 90, 103.6, 90], 'no'], 'Crocidolite_whittaker_1949': ['Crocidolite_whittaker_1949', [9.89, 17.85, 5.31, 90, 107.5, 90],*

Simulation of orientation or deformation gradient. From parent grain simulate a list of transformations (deduced by a parametric variation)

_list_param : list of parameters for each grain [grain parameters, grain name]

posCEN =(Xcen, Ycen) cameraAngles =(Xbet, Xgam)

Returns (list_twicetheta, list_chi, list_energy, list_Miller, list_posX, list_posY, ParentGrainName_list, list_ParentGrain_transforms, calib, total_nb_grains)

TODO:simulate for any camera position TODO: simulate spatial distribution of laue pattern origin

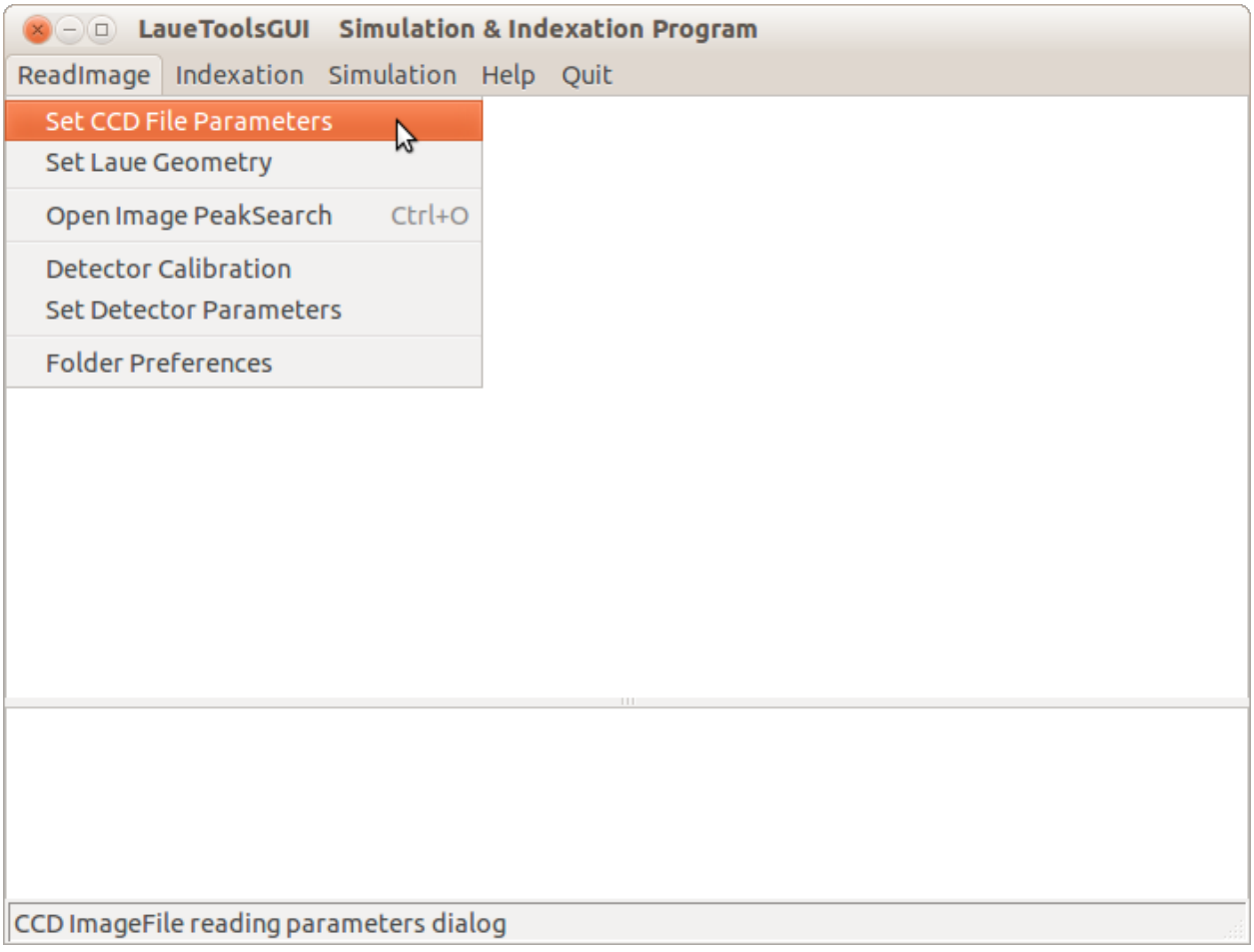
7.3 Modules for Digital Image processing, Peak Search & Fitting

7.3.1 PeakSearchGUI

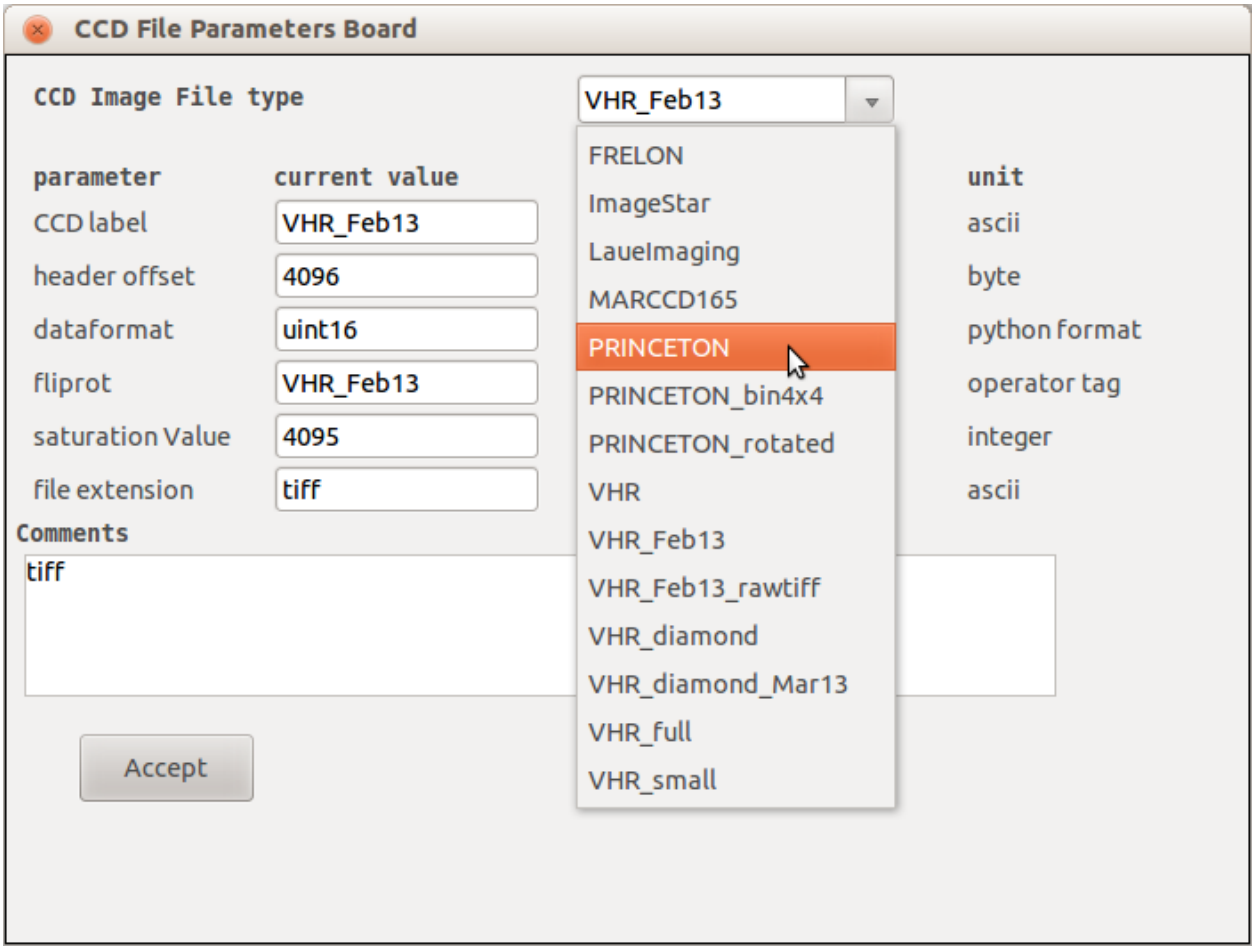
The module PeakSearchGUI.py is made to provide graphical tools to perform peak search and fitting. It enables also tools to get mosaic from a set of images.

Read Images and Binary files

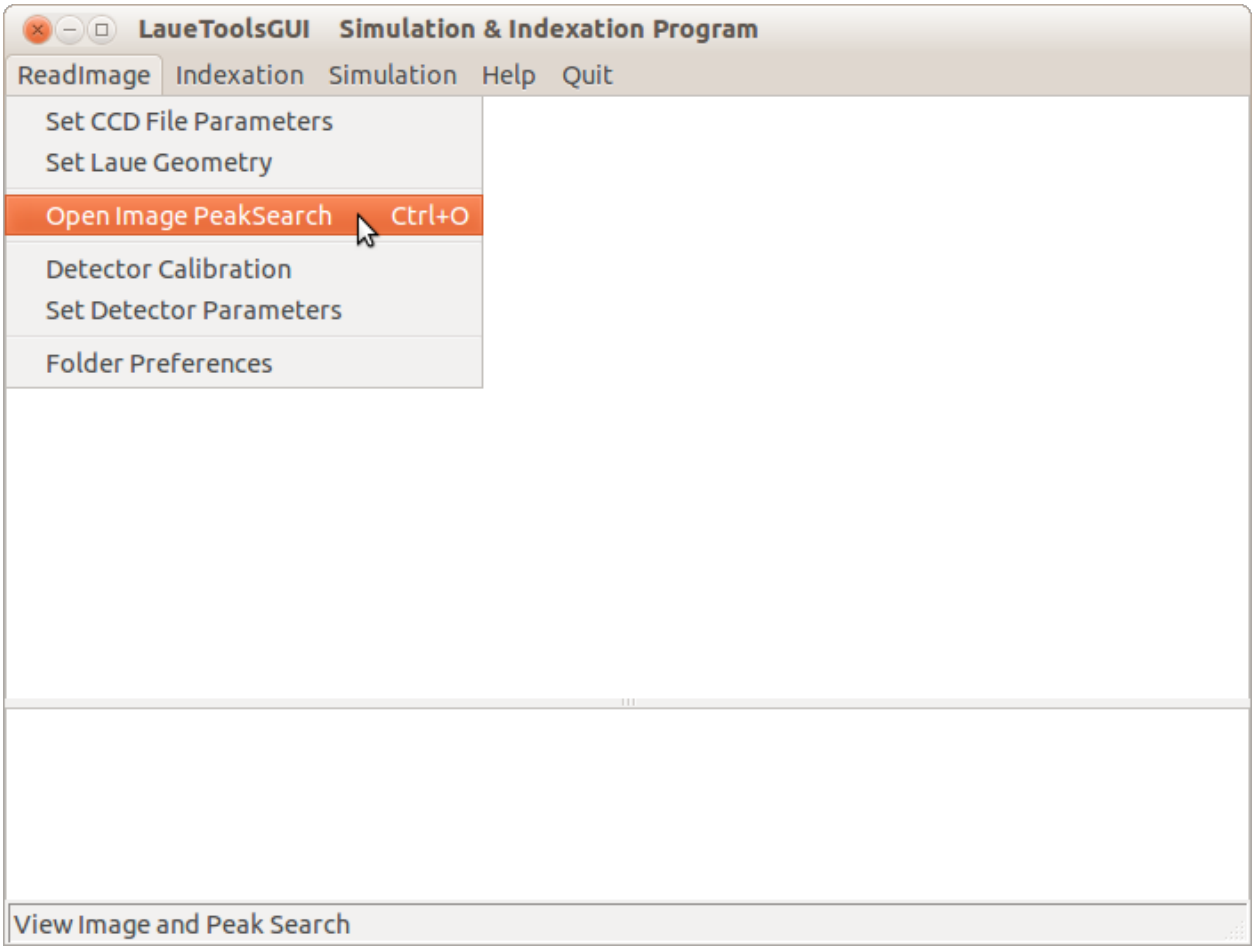
First select the detector you have used for the data collection in the menu Calibration



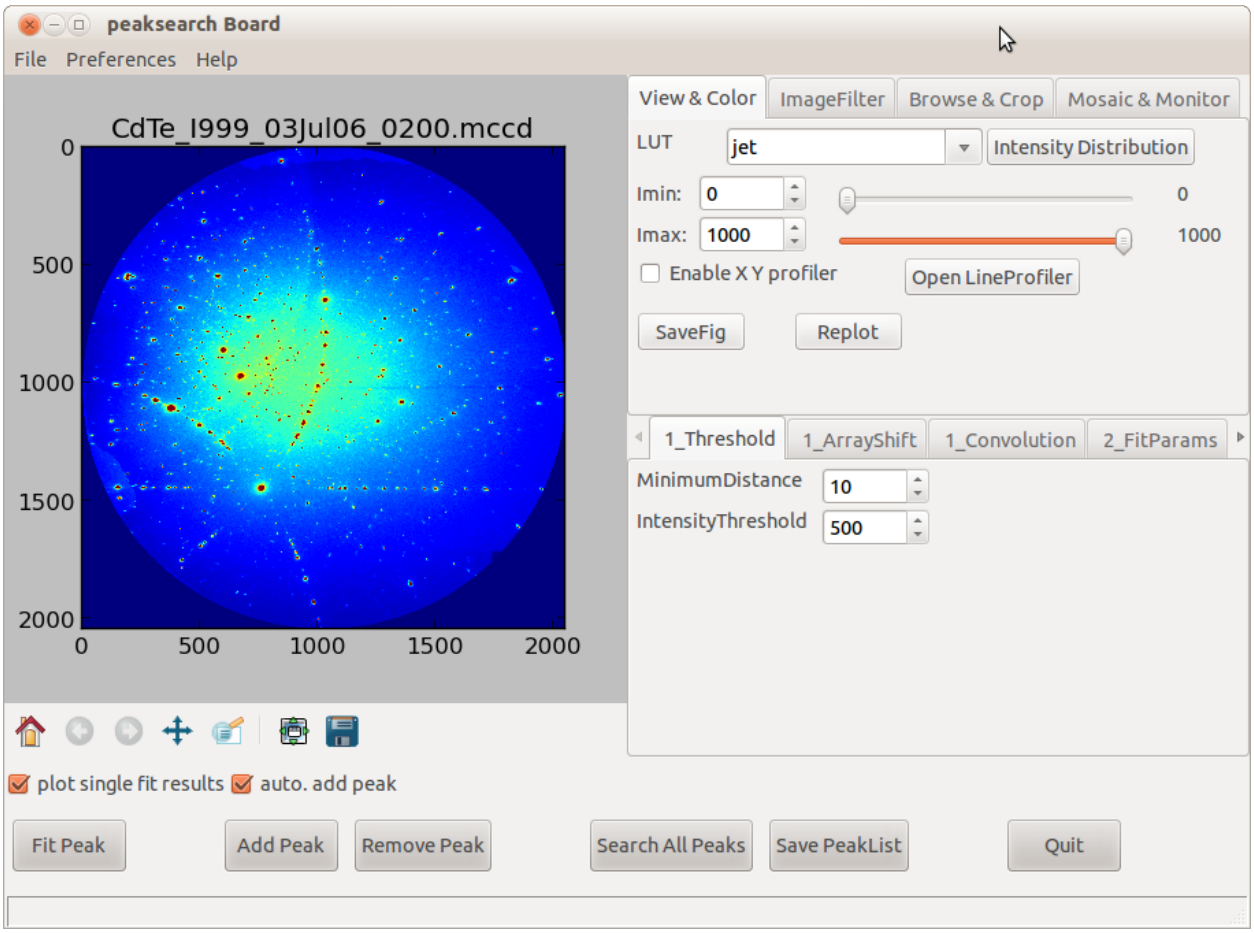
Choose the correct camera to define the binary image file parameters



View an image by selecting in the Menu File/Open Image and Peak Search.



Then you obtain a board enabling to browse your set of images and to search for peaks



This board is composed by composed by 4 TOP tabs:

- parameters of display (View & color)
- Digital image processing (Image & Filter)
- Browse a set of images and select a ROI (Browse & crop)
- Mosaic or image-related monitor from a ROI over a set of images

And 5 tabs at the middle

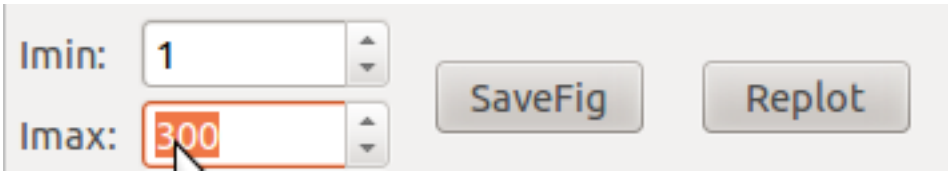
- 1 Selection of local maxima search Method
- 2 Fitting procedure parameters
- 3 Peaks List Manager

View & Color

This panel helps for viewing images with an appropriate color LUT, getting some infos on pixels intensity on the whole image (distribution) or along line (line profilers)

- Color Mapping (LUT) of the displayed image. `ShowHisto` displays the histogram of intensity distribution (nb of pixel as a function of pixel intensity)

- intensities limits taken into account by the LUT



- `Open LineProfiler`: 1D plot of pixel intensities along a movable-by-user line. And `Eneable X Y Profiler`: 1D plot of pixel intensities along X and Y from a clicked pixel position

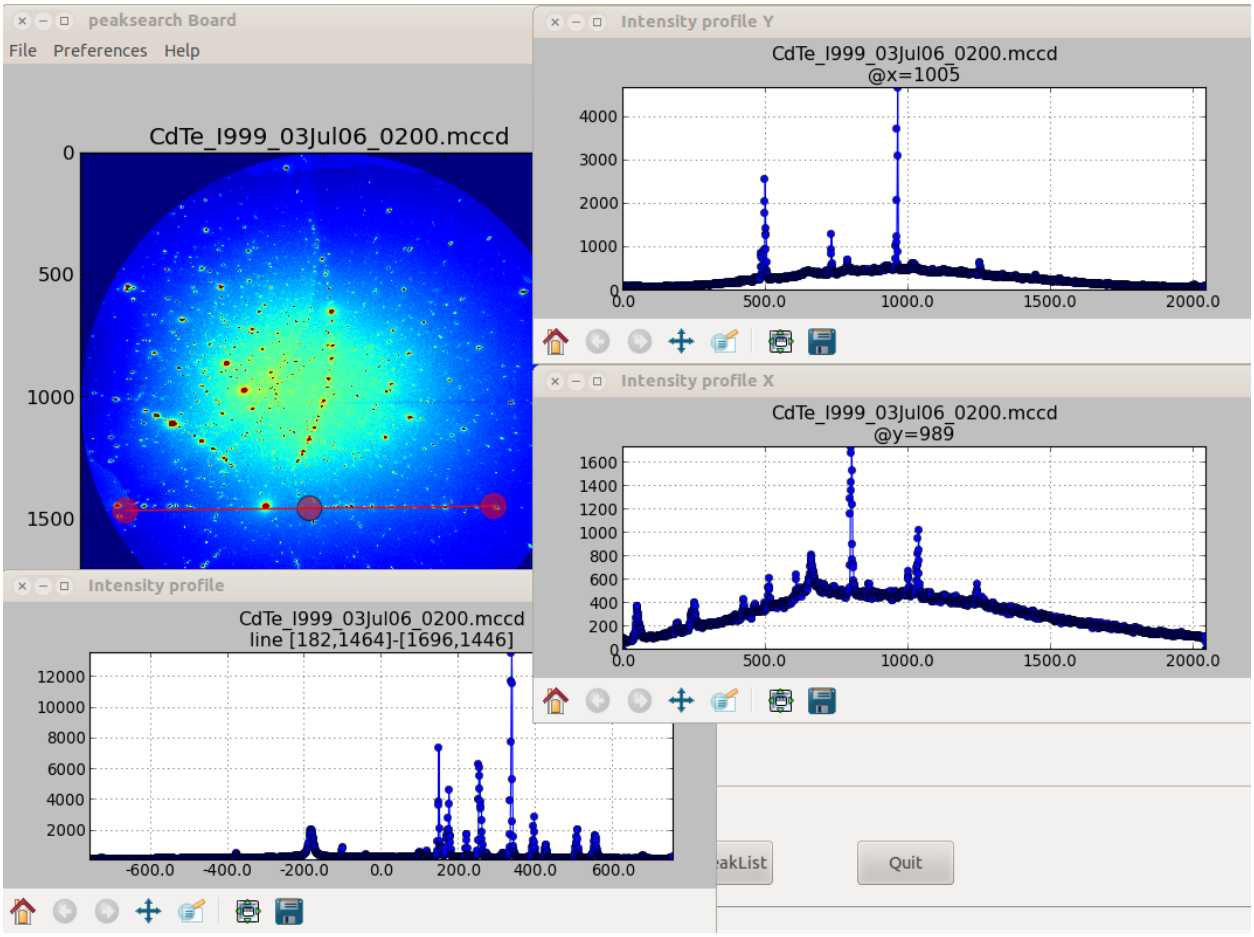


Image & Filter

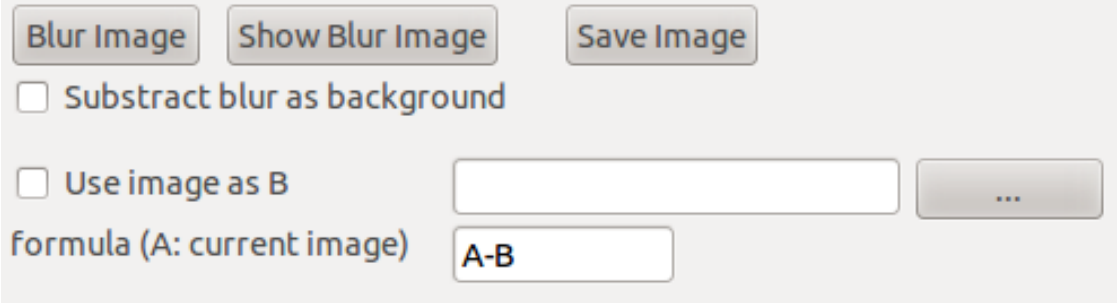
This panel supplies digital image processing tools to filter current image and particularly remove background.

`Blur Image` computes the image filtered by a gaussian kernel (similar to a low pass filter). By checking `Substract blur as background` the raw image minus the filtered image can be displayed and used for the local maxima (blob) search.

`Calculate image with A and B` allows with an arithmetical formula with A (current image) and B (addi-

tional image to be open) the computation of a new image A' on which will be performed the local maxima (blob) searchChecking. By default this image will not be used to refine the position and shape of local maxima but the former and initial A image. Check `use also for fit` to apply the fit procedures on pixel intensities A'.

`Save results` saves on hard disk the A' image with the header contains and format of A.

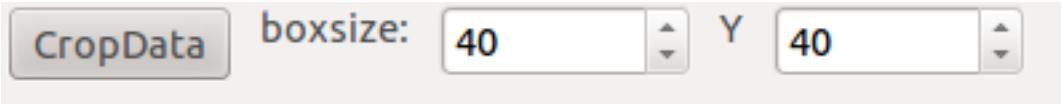


Browse & Crop

One can navigate on a set of images provided the images file name contains a numerical index with a constant prefix (e.g. myimage_0032.ccd). Navigation with button with small step `index-1` and `index+1` corresponds to consecutive images collected with time or along a line on sample. Navigation with button with larger step (Nb of images per line (step index)) `index-10` and `index+10` (for instance with larger step equals to 10) permits to look at the images collected along the direction perpendicular to the direction corresponding to the small step.

The `Go To index` button allows to read directly an image with an other in the same dataset. `Auto index+1` button will display the next image and wait for it if it is not already in the folder.

To navigate and display faster the image when browsing on a particular region of interest (ROI) of the images, you can crop the data (`CropData`) by specifying the half sizes (`boxsize`) of the cropping box in the two directions.



Mosaic & Monitor

Several counters can be defined from pixel intensities in the same ROI (centered a clicked pixel with half box sizes given by user) over a set of images.

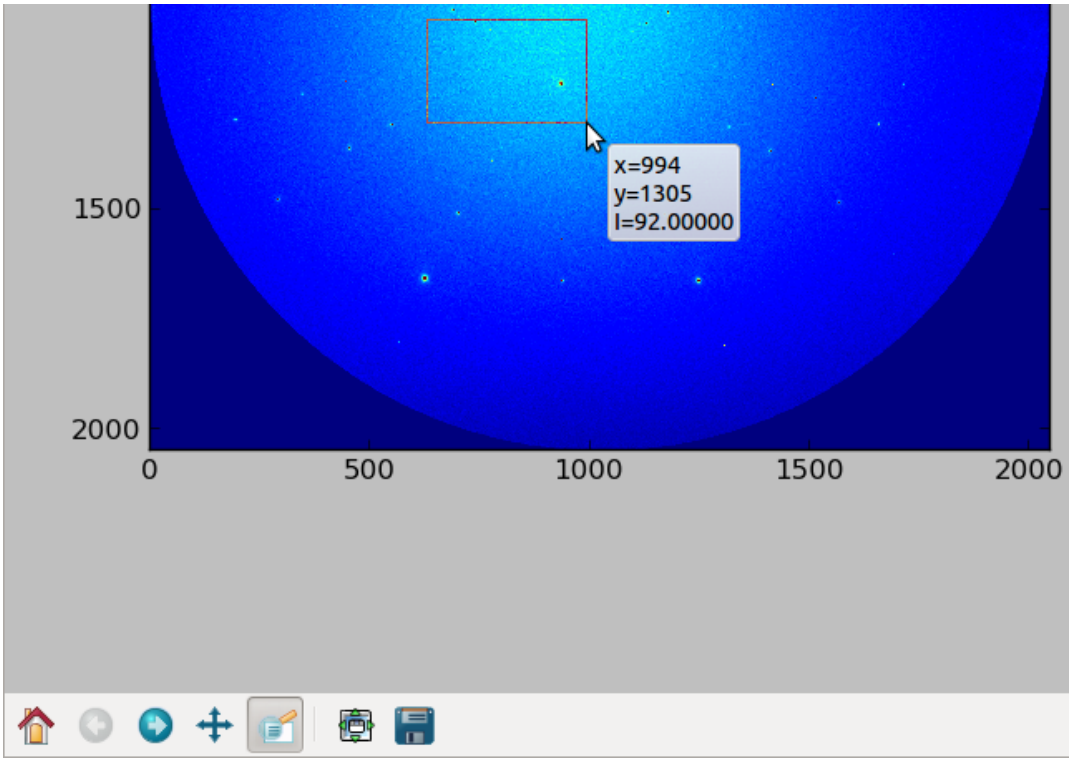
- Mosaic: Recompose a 2D raster scan from the selected ROI of each images as a function of image index
- Mean Value: plot a 1D graph or a 2D raster scan from the mean pixel value in the selected ROI of each images as a function of image index

- Max Value: plot a 1D graph or a 2D raster scan from the maximum pixel value in the selected ROI of each images as a function of image index
- Peak-to-peak Value (or 'peak to valley'): plot a 1D graph or a 2D raster scan from the largest pixel amplitude value in the selected ROI of each images as a function of image index
- Peak position: plot two 1D graphes of X and Y peak position of the peak in the selected ROI of each images as a function of image index

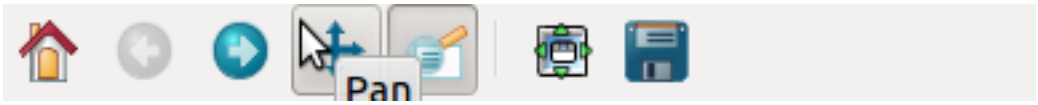
Plot Tools

The standard toolbar is provided by the graphical 'matplotlib' library with the following features:

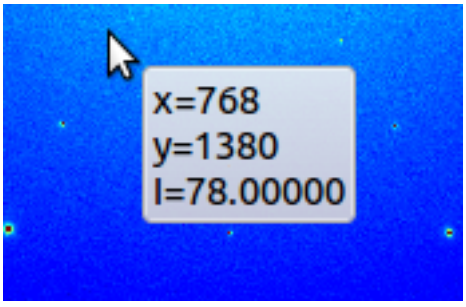
- A ROI can be set to zoom in the data.



- This ROI can be moved easily with the pan button



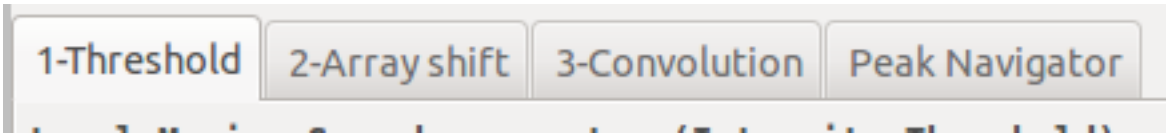
- When hovering the mouse on the image pixel position and corresponding intensity are displayed



- Previous selected ROIs are stored and can be recalled by arrows (`Home` icon recalls the initial full image)

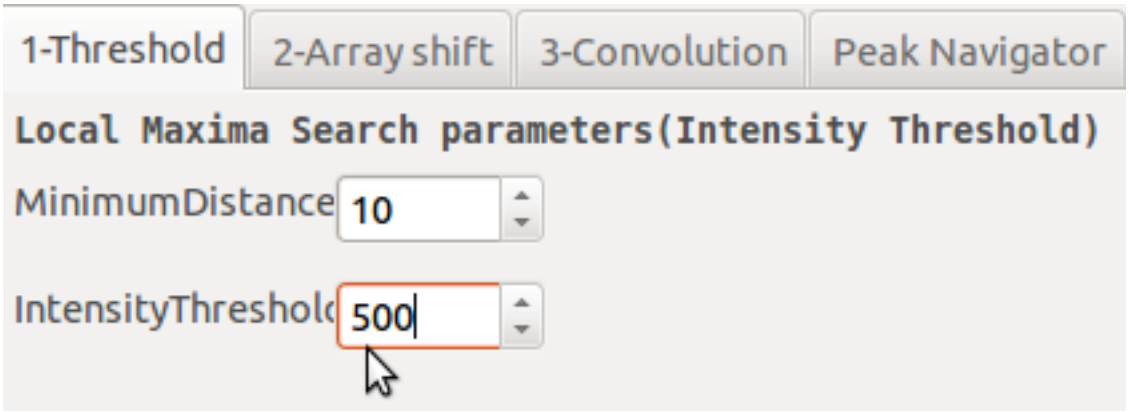
Local Maxima or Blob Search

To guess the initial parameters fitting, 3 methods leads to a list of local maxima (or blobs)



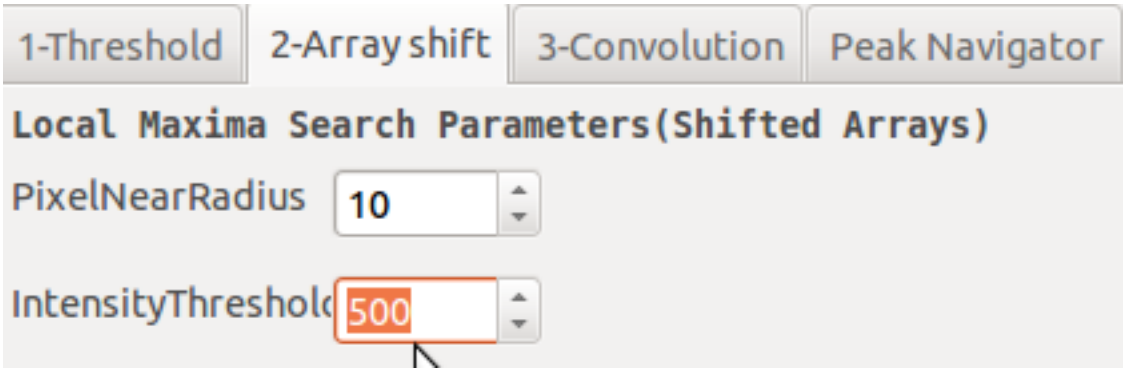
Method 1: pixels above a threshold on raw image

The basic method consists in considering every pixel higher than `intensityThreshold` as a local maxima pixel. If `intensityThreshold` is too high you will get only few pixels at the submit of laue spots. If `intensityThreshold` is too small you will too much pixels that you may stuck the software. `MinimumDistance` is the smallest distance separating two local maxima. A good habit is too check the highest background level (e.g close to the image centre) and set `intensityThreshold` to a larger value. But even in this case if (fluorescence) background varies a lot, you will miss peaks whose maximum intensities are below the threshold... This is why removing the background is mandatory.



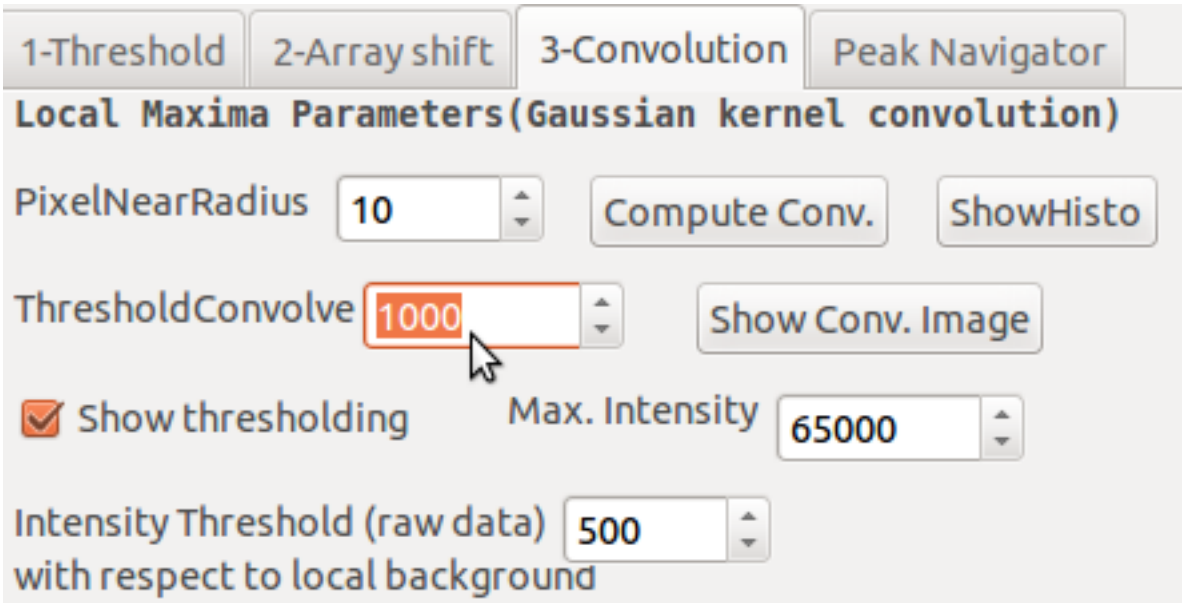
Method 2: hottest pixel in a box (by array shift)

Second Method finds the hottest pixel in a small box given by `PixelNearRadius`. It shifts the whole data array in 8 directions and determines every pixel hotter than the others lying in these 8 directions. The **thresholding** with the `IntensityThreshold` level is performed on the intensity of these hot pixels **with respect to local background level** (set to the lowest pixel intensity in the box around the hot pixel). One drawback of this method is that 2 hot pixels at the top of the peak but with strictly the same intensity are not detected (coincidence or more likely when peak is saturated).



Method 3: Peak enhancement by convolution on raw image

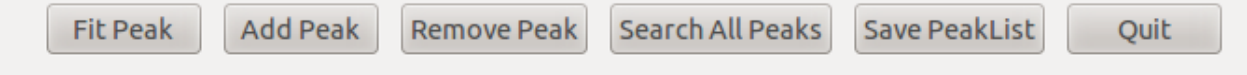
This is the fastest method as soon as you have found the few parameters value (for batch). The *Raw image* data (unsigned 16 bits integers) are convolved by a 2D gaussian (mexican-hat-like) kernel. The resulting *convolved Image* (floats) have intense region (called blobs) where pixel intensity 2D profile on raw data is similar to the kernel intensity profile. A first threshold with the level `ThresholdConvolve` (float) allows to select enhanced blob above a background. An good estimate of `ThresholdConvolve` value can be found by means of the pixel intensity histogram (`ShowHisto`): it corresponds to the (float) intensity that separates the hottest pixel population that belong to the peak (large abscisssa value) from the weakest one that belong to background. With this blobs list, a second thresholding at `Intensity Threshold (raw data)` level is performed in the raw data pixel intensity with respect to local background level (like in method 2). `PixelNearRadius` value enables the user to reject too much closed spots. `Max.Intensity` value is used for the display of the convolved Image by clicking on `Show Conv. Image`. Thresholding can be visualize by checking `Show thresholding`.



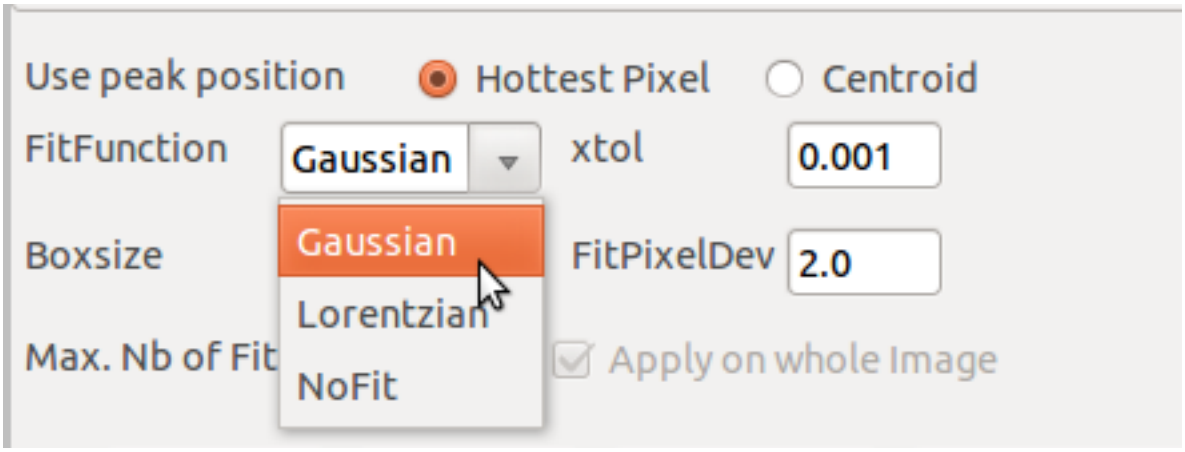
Peak Position Fit

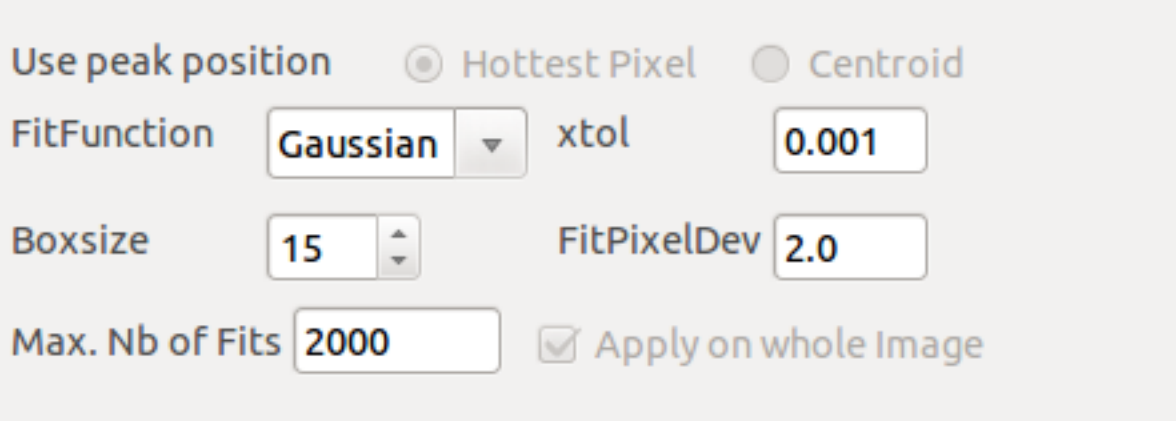
The goal of the peak search is to have systematic values of Laue peaks and intensities. You can decide to fit or not the blob found. The Button `Search All Peaks` launches the local maxima chosen method and apply a fitting procedure (or not) to each found blob. A general peak list is built. By clicking close to a Laue spot in the image and clicking on the `Fit Peak` button, a gaussian fit is performed. This result can be added to the current general peak

list with the button `Add Peak`. Clicking close to a Laue spot that belongs to the peak list (blue circle marker on top of the image) and pressing `Remove Peak` removes the laue spot from the list.



Parameters to choose the fitting model or no fit and to reject or not the fitting result of each peak according to deviation from the initial guessed position (`FitPixelDeviation`).





Module functions

The next documentation comes from the docstring in the header of function or class definition.

PeakSearchGUI.py (PeakSearchBoard)

class `LaueTools.GUI.PeakSearchGUI.`**ViewColorPanel**(*parent*)

class to play with color LUT and intensity scale

OnReplot(_)

trigger main self.mainframe.OnReplot(1)

getclickposition(*event*)

return closest pixel integer coordinates to clicked pt

OnShowLineXYProfiler(*event*)

show line X and Y profilers

bestposition(*LINEPROFILE_WIDTH*, *LINEPROFILE_HEIGHT*)
return xp, yp (best position)

restrictxylimits_to_imagearray(*xmin*, *ymin*, *xmax*, *ymax*)
return compatible extremal value of x,y xmin, ymin, xmax, ymax

getlineprofiledata(*x0*, *y0*, *x2*, *y2*)
get pixel intensities array between two points (x0,y0) and (x2,y2)

return dataX, dataY

OnShowLineProfiler(_)
show a movable and draggable line profiler and draw line and circle

updateLineXYProfile(*event*)
recompute line section intensity profile horizontal (x, zx) vertical (y, zy)

onOpenDetFile(_)
open and read .det file with geometry detection calibration parameters

set self.DetFilename set self.mainframe.DetFilename

showImage()
branching from button of ViewColorPanel class: show blur/raw image

class LaueTools.GUI.PeakSearchGUI.**FilterBackGroundPanel**(*parent*)
class to handle image background tools

Computefilteredimage()
remove background if self.blurimage exists

onComputeBlurImage(_)
Compute background, blurred, filtered or low frequency spatial image from current image

set self.blurimage

OnSwitchBlurRawImage(_)
set viewing of raw image (- background) or background (=filtered image)

onSaveBlurImage(_)
save on hard disk blurred or background image obtained from current image

onSaveFormulaResultImage(_)
save image on hard disk of data obtained by arithmetical formula

onGetBImagefilename(_)
open image as B image set self.BImageFilename

onGetBlackListfilename(_)
open black peakslist file set self.BlackListFilename set self.mainframe.BlackListFilename

OnChangeUseFormula(*evt*)
change arithmetical formula

class LaueTools.GUI.PeakSearchGUI.**BrowseCropPanel**(*parent*)
class to handle crop operation on images

class LaueTools.GUI.PeakSearchGUI.**MosaicAndMonitor**(*parent*)

OnMosaic(_)
launch main procedure of computing mosaic and displaying it

class LaueTools.GUI.PeakSearchGUI.**ROISelection**(*parent*)

onCenterROI(*evt*)
simply click and later press q

class LaueTools.GUI.PeakSearchGUI.**PlotPeakListPanel**(*parent*)
panel class to handle peaks list within GUI

OnShowLineXYProfiler(*event*)
show line X and Y profilers

getlineprofiledata(*x0*, *y0*, *x2*, *y2*)
get pixel intensities array between two points (x0,y0) and (x2,y2)

OnShowLineProfiler(_)
show a movable and draggable line profiler and draw line and circle

class LaueTools.GUI.PeakSearchGUI.**findLocalMaxima_Meth_1**(*parent*)
class of method 1 for local maxima search (intensity threshold)

class LaueTools.GUI.PeakSearchGUI.**findLocalMaxima_Meth_2**(*parent*)
class of method parameters for 2nd method of local maxima(shifted arrays)

class LaueTools.GUI.PeakSearchGUI.**findLocalMaxima_Meth_3**(*parent*)
class of method 3 for local maxima search (convolution by a mexican hat kernel)

OnSwitchImageDisplay(*evt*)
switch between raw and convolved image display (performed by MainPeakSearchFrame class)

class LaueTools.GUI.PeakSearchGUI.**FitParametersPanel**(*parent*)

class LaueTools.GUI.PeakSearchGUI.**PeakListOLV**(*parent*)
panel embedding an ObjectListViewer from ObjectListView module

need of: self.grangranparent.peaklistPixels self.grangranparent.onRemovePeaktoPeaklist self.grangranparent.OnReplot self.grangranparent.framedim and lot of other things with mainframe...

OnRemove(_)
remove one element corresponding to the current highlighted row

class LaueTools.GUI.PeakSearchGUI.**MainPeakSearchFrame**(*parent*, *_id*, *_initialParameter*, *title*, *size=4*)
Class to show CCD frame pixel intensities and provide tools for searching peaks

create_main_panel()
Creates the main panel with all the controls on it: * mpl canvas * mpl navigation toolbar * Control panel for interaction

toplayout2()
init top notebook tabs for image visualisation and processing

line_select_callback(*eclick*, *erelease*)
eclick and erelease are the press and release events

OnTabChange_nb0(*event*)
handling changing tab of top notebook

askUserForDirname()
provide a dialog to browse the folders and files

OnSetFileCCDParam(_)
Enter manually CCD file params Launch Entry dialog

OnSetPlotSize(_)
set marker size

onClick(*event*)
onclick

onKeyPressed(*event*)
Handle key pressed

gettime()
set self.currentime to current time

onToggle(*event*)
handling on auto index button

onToggleCrop(*event*)
activate/deactivate crop image mode

update(_)
update at each time step time

CurrentFileIsReady()
return True if self.imagefilename is in folder and entire (correct size)

getIndex_fromfilename()
get index of image from the image filename

setfilename()
set filename from self.imagefilename, self.imageindex, CCDLabel=self.CCDlabel

OnLargePlus(_)
increase self.imageindex by self.stepindex (vertical descending in sample raster scan) and read new image and plot

OnLargeMinus(_)
decrease self.imageindex by self.stepindex (vertical ascendindg in sample raster scan) and read new image and plot

OnPlus(_)
increase self.imageindex by 1 (horizontal ascending to the right in sample raster scan) and read new image and plot

OnMinus(_)
decrease self.imageindex by 1 (horizontal descending to the left in sample raster scan) and read new image and plot

OnGoto(_)
read image with selected self.imageindex and plot

onChangeIndex_slider_imagevert(_)
plot new image obtained by new index changed by vertical (slow axis) slider

read_data(*secondaryImage=False*, *secondaryImagefilename=None*)
read binary image file

if secondaryImage update self.dataimage_ROI_B

else update self.dataimage_ROI

OnCheckPlotValues(_)
enable or disable drawing of numerical pixel intensity value on plot

PlotValues()
Draw numerical pixel intensity value on plot

init_figure_draw()
init the figure

Show_Image(*event*, *datatype='Raw Image'*)
show self.dataimage_ROI_display

Show_ConvolvedImage(*event*, *datatype='Convolved Image'*)
set displayed data to be convolved data

updatePlotTitle(*datatype=None*)
update plot title

normalizeplot()
normalize current displayed array according to vmin vmax sliders

update_draw(_)
update 2D plot taken into account change of LUT table and vmin vamax values

getDisplayedImageSize()
get xmin, xmax, ymin, ymax from current displayed image

set_circleradius(*self.viewingLUTpanel.drg.artists*)

activateCrop(_)
set boxx and boxy from ctrls

readdata_updateplot_aftercrop_uncrop()
read data and update data to be displayed and redraw

reinit_aftercrop_draw()
reinit the figure

buildMosaic(*parent=None*)
launch MOS.buildMosaic3() with GUI inputs as arguments

onMotion_ToolTip(*event*)
tool tip to show data when mouse hovers on plot Some pixels at the image border could not be detected

OnSpinCtrl_ImaxDisplayed(*event*)
on change Imax by spin control

Get_XYI_from_fit2dpeaksfile(*filename*)
useless ?

draw_cursor(*event*)
event is a MplEvent. Draw a cursor over the axes

getConvolvedData()
convolve data according to check value of

SavePeakList_PSPfile(_)
save peak list and save .psp file

onSaveROIsList(_)
save rois list from current peaks list with boxsize of fitting procedure

onFitOnePeak(_)
fit one peak centered on where user has clicked

in displayed image coordinates: self.centerx, self.centery

OnFit()
fit image array in a ROI with a 2D gaussian shape

onRemovePeaktoPeaklist(_, *centerXY=None*)
remove picked peak from the current peaks list

onRemoveAllPeakstoPeaklist(_)
remove all spots of the peaks list and update the plot (remove circular markers)

getClosestPeak(*centerXY=None*)
return peak in self.peaklistPixels that is close to the clicked pixel position or the given value

deleteOnePeak(*index_close*, *peakXY*)
delete one peak and update display and lists

deleteAllPeaks()
delete all peaks and update display and lists

OnPeakSearch(_)
launch peak search by calling methods in readmccd.py

7.3.2 Peak Search and Fit (readmccd.py)

Module functions

The next documentation comes from the docstring in the header of function or class definition.

readmccd.py

readmccd module is made for reading data contained in binary image file fully or partially. It can process a peak or blob search by various methods and refine the peak by a gaussian or lorentzian 2D model

More tools can be found in LaueTools package at sourceforge.net and gitlab.esrf.fr

LaueTools.readmccd.**setfilename**(*imagefilename*, *imageindex*, *nbdigits=4*, *CCDLabel=None*)
reconstruct filename string from imagefilename and update filename index with imageindex

Parameters

- **imagefilename** – filename string (full path or not)
- **imageindex** (*string*) – index in filename

Return filename input filename with index replaced by input imageindex

Return type string

LaueTools.readmccd.**getIndex_fromfilename**(*imagefilename*, *nbdigits=4*, *CCDLabel=None*, *stackimageindex=-1*)
get integer index from imagefilename string

Parameters **imagefilename** – filename string (full path or not)

Returns file index

LaueTools.readmccd.**readheader**(*filename*, *offset=4096*, *CCDLabel='MARCCD165'*)
return header in a raw format

default offset for marccd image

LaueTools.readmccd.**read_header_marccd**(*filename*)
return string of parameters found in header in marccd image file .mccd

- print allsentences displays the header
- use allsentences.split('n') to get a list

LaueTools.readmccd.**read_header_marccd2**(*filename*)
return string of parameters comments and exposure time found in header in marccd image file .mccd

- print allsentences displays the header
- use allsentences.split('n') to get a list

LaueTools.readmccd.**read_header_scmos**(*filename*)
return string of parameters comments and exposure time found in header in scmis image file .tif

- print allsentences displays the header
- use allsentences.split('n') to get a list

LaueTools.readmccd.**readCCDimage**(*filename*, *CCDLabel='MARCCD165'*, *dirname=None*, *stackimageindex=-1*, *verbose=0*)
Read raw data binary image file.

Read raw data binary image file and return pixel intensity 2D array such as to fit the data (2theta, chi) scattering angles representation convention.

Parameters

- **filename** (*str*) – path to image file (fullpath if ' dirname' =None)
- **CCDLabel** (*str, optional*) – label, defaults to "MARCCD165"
- **dirname** (*str, optional*) – folder path, defaults to None
- **stackimageindex** (*int, optional*) – index of images bunch, defaults to -1
- **verbose** (*int, optional*) – 0 or 1, defaults to 0

Raises **ValueError** – if data format and CCD parameters from label are not compatible

Returns

- dataimage, 2D array image data pixel intensity properly oriented
- framedim, iterable of 2 integers shape of dataimage
- fliprot : string, key for CCD frame transform to orient image

Return type tuple of 3 elements

LaueTools.readmccd.**readoneimage**(*filename*, *framedim=(2048, 2048)*, *dirname=None*, *offset=4096*, *formatdata='uint16'*)
returns a 1d array of integers from a binary image file (full data)

Parameters

- **filename** (*str*) – image file name (full path if dirname=0)
- **framedim** (*tuple of 2 integers, optional*) – detector dimensions, defaults to (2048, 2048)
- **dirname** (*str, optional*) – folder path, defaults to None
- **offset** (*int, optional*) – file header in byte (octet), defaults to 4096
- **formatdata** (*str, optional*) – numpy format of raw binary image pixel value, defaults to "uint16"

Returns dataimage : image data pixel intensity

Return type 1D array

LaueTools.readmccd.**readoneimage_crop_fast**(*filename*, *dirname=None*, *CCDLabel='MARCCD165'*, *firstElemIndex=0*, *lastElemIndex=2047*)

Returns a 2d array of integers from a binary image file. Data are taken only from a rectangle

with respect to firstElemIndex and lastElemIndex.

Parameters

- **filename** – string, path to image file (fullpath if ' dirname'=None)
- **offset** – integer, nb of file header bytes
- **framedim** – iterable of 2 integers, shape of expected 2D data
- **formatdata** – string, key for numpy dtype to decode binary file

Returns dataimage : 1D array image data pixel intensity

LaueTools.readmccd.**readrectangle_in_image**(*filename*, *pixx*, *pixy*, *halfboxx*, *halfboxy*, *dirname=None*, *CCDLabel='MARCCD165'*, *verbose=True*)

returns a 2d array of integers from a binary image file. Data are taken only from a rectangle centered on pixx, pixy

Returns dataimage : 2D array, image data pixel intensity

LaueTools.readmccd.**readoneimage_crop**(*filename*, *center*, *halfboxsize*, *CCDLabel='PRINCETON'*, *dirname=None*)

return a cropped array of data read in an image file

Parameters

- **filename** – string, path to image file (fullpath if ' dirname'=None)
- **center** – iterable of 2 integers, (x,y) pixel coordinates
- **halfboxsize** – integer or iterable of 2 integers, ROI half size in both directions

Returns dataimage : 1D array, image data pixel intensity

#TODO: useless?

LaueTools.readmccd.**readoneimage_manycrops**(*filename*, *centers*, *boxsize*, *stackimageindex=-1*, *CCDLabel='MARCCD165'*, *addImax=False*, *use_data_corrected=None*)

reads 1 image and extract many regions centered on center_pixel with xyboxsize dimensions in pixel unit

Parameters filename : string,fullpath to image file centers : list or array of [int,int] centers (x,y) pixel coordinates use_data_corrected : enter data instead of reading data from file

must be a tuple of 3 elements: fulldata, framedim, fliprot where fulldata is a numpy.ndarray as output by *readCCDimage()*

boxsize [iterable 2 elements or integer] boxsizes [in x, in y] direction or integer to set a square ROI

Returns Data : list of 2D array pixel intensity

Imax : returns: array of data: list of 2D array of intensity

LaueTools.readmccd.**readoneimage_multiROIfit**(*filename*, *centers*, *boxsize*, *stackimageindex=-1*, *CCDLabel='PRINCETON'*, *baseline='auto'*, *startangles=0.0*, *start_sigma1=1.0*, *start_sigma2=1.0*, *position_start='max'*, *fitfunc='gaussian'*, *showfitresults=1*, *offsetposition=0*, *verbose=0*, *xtol=1e-08*, *addImax=False*, *use_data_corrected=None*)

Fit several peaks in one image

Parameters filename : string, full path to image file centers : list or array like with shape=(n,2)

list of centers of selected ROI

boxsize [(Truly HALF boxsize: fuill boxsize= 2 *halfboxsize +1)] iterable 2 elements or integer boxsizes [in x, in y] direction or integer to set a square ROI

Optional parameters baseline : string

'auto' (ie minimum intensity in ROI) or array of floats

startangles [float or iterable of 2 floats] elliptic gaussian angle (major axis with respect to X direction), one value or array of values

start_sigma1, start_sigma2: floats gaussian standard deviation (major and minor axis) in pixel,

position_start [string] starting gaussian center:'max' (position of maximum intensity in ROI), 'centers' (centre of each ROI)

offsetposition [integer] 0 for no offset 1 XMAS compatible, since XMAS consider first pixel as index 1 (in array, index starts with 0) 2 fit2d, since fit2d for peaksearch put pixel labelled n at the position n+0.5 (between n and n+1)

use_data_corrected [tuple of 3 elements] Enter data instead of reading data from file: fulldata, framedim, fliprot where fulldata is a ndarray

returns params_sol : list of results

bkg, amp (gaussian height-bkg), X , Y ,

major axis standard deviation ,minor axis standard deviation, major axis tilt angle / Ox

TODO: setting list of initial guesses can be improve with scipy.ndimages of a concatenate array of multiple slices?

LaueTools.readmccd.**getindices2cropArray**(*center*, *halfboxsizeROI*, *arrayshape*, *flipxycenter=False*)

return array indices limits to crop array data

Parameters center : iterable of 2 elements

(x,y) pixel center of the ROI

halfboxsizeROI [integer or iterable of 2 elements] half boxsize ROI in two dimensions

arrayshape [iterable of 2 integers] maximal number of pixels in both directions

Options flipxycenter : boolean

True: swap x and y of center with respect to others parameters that remain fixed

Return imin, imax, jmin, jmax : 4 integers

4 indices allowing to slice a 2D np.ndarray

Todo: merge with check_array_indices()

LaueTools.readmccd.**check_array_indices**(*imin*, *imax*, *jmin*, *jmax*, *framedim=None*)
Return 4 indices for array slice compatible with framedim

Parameters imin, imax, jmin, jmax: 4 integers

mini. and maxi. indices in both directions

framedim [iterable of 2 integers] shape of the array to be sliced by means of the 4 indices

Return imin, imax, jmin, jmax: 4 integers

mini. and maxi. indices in both directions

Todo: merge with getindices2cropArray()

LaueTools.readmccd.**to8bits**(*PILimage*, *normalization_value=None*)
convert PIL image (16 bits) in 8 bits PIL image returns: [0] 8 bits image [1] corresponding pixels value array

TODO: since not used, may be deleted

LaueTools.readmccd.**writeimage**(*outputname*, *_header*, *data*, *dataformat=<class 'numpy.uint16'>*)
from data 1d array of integers with header coming from a f.open('imagefile'); f.read(headersize);f.close() WARNING: header contain dimensions for subsequent data. Check before the compatibility of data with header infos(nb of byte per pixel and array dimensions

LaueTools.readmccd.**write_rawbinary**(*outputname*, *data*, *dataformat=<class 'numpy.uint16'>*)
write a binary file without header of a 2D array

LaueTools.readmccd.**SumImages**(*prefixname*, *suffixname*, *ind_start*, *ind_end*, *dirname=None*, *plot=0*, *output_filename=None*, *CCDLabel=None*, *nbdigits=0*)
sum images and write image with 32 bits per pixel format (4 bytes)

LaueTools.readmccd.**Add_Images**(*prefixname*, *ind_start*, *ind_end*, *plot=0*, *writefilename=None*)
Add continuous sequence of images

Note: Add_Images2 exists

Parameters prefixname : string

prefix common part of name of files

ind_start [int] starting image index

ind_end [int] final image index

Optional Parameters writefilename: string

new image filename where to write datastart (with last image file header read)

Returns datastart : array

accumulation of 2D data from each image

LaueTools.readmccd.**diff_pix**(*pix*, *array_pix*, *radius=1*)
returns index in array_pix which is the closest to pix if below the tolerance radius

array_pix: array of 2d pixel points pix: one 2elements pixel point

LaueTools.readmccd.**getExtrema**(*data2d*, *center*, *boxsize*, *framedim*, *ROIcoords=0*, *flipxycenter=True*)
return min max XYposmin, XYposmax values in ROI

Parameters ROIcoords : 1 in local array indices coordinates

0 in X,Y pixel CCD coordinates

flipxycenter [boolean like] swap input center coordinates

data2d [2D array] data array as read by *readCCDimage()*

Return min, max, XYposmin, XYposmax:

- min : minimum pixel intensity
- max : maximum pixel intensity
- XYposmin : list of absolute pixel coordinates of lowest pixel
- XYposmax : list of absolute pixel coordinates of largest pixel

LaueTools.readmccd.**getIntegratedIntensities**(*fullpathimagefile*, *list_centers*, *boxsize*, *CCDLabel='MARCCD165'*, *thresholdlevel=0.2*, *flipxycenter=True*)
read binary image file and compute integrated intensities of peaks whose center is given in list_centers

return array of column 0: integrated intensity column 1: absolute minimum intensity threshold column 2: nb of pixels composing the peak

LaueTools.readmccd.**getIntegratedIntensity**(*data2d*, *center*, *boxsize*, *framedim*, *thresholdlevel=0.2*, *flipxycenter=True*)
return crude estimate of integrated intensity of peak above a given relative threshold

Parameters ROIcoords : 1 in local array indices coordinates

0 in X,Y pixel CCD coordinates

flipxycenter [boolean like] swap input center coordinates

data2d [2D array] data array as read by *readCCDimage()*

Thresholdlevel [relative level above which pixel intensity must be taken into account] I(p)- minimum> Thresholdlevel* (maximum-minimum)

Return integrated intensity, minimum absolute intensity, nbpixels used for the summation

LaueTools.readmccd.**getMinMax**(*data2d*, *center*, *boxsize*, *framedim*)
return min and max values in ROI

Parameters:

data2d [2D array] array as read by readCCDimage

LaueTools.readmccd.**LoGArr**(*shape=(256, 256)*, *r0=None*, *sigma=None*, *peakVal=None*, *orig=None*, *wrap=0*, *dtype=<class 'numpy.float32'>*)
returns n-dim Laplacian-of-Gaussian (aka. mexican hat) if peakVal is not None

result max is peakVal

if r0 is not None: specify radius of zero-point (IGNORE sigma !!)

credits: "Sebastian Haase <haase@msg.ucsf.edu>"

LaueTools.readmccd.**ConvolvebyKernel**(*Data*, *peakVal=4*, *boxsize=5*, *central_radius=2*)

Convolve Data array witn mexican-hat kernel

inputs: Data : 2D array containing pixel intensities peakVal > central_radius : defines pixel distance from box center where weights are positive

(in the middle) and negative farther to converge back to zero

boxsize : size of the box

ouput: array (same shape as Data)

LaueTools.readmccd.**LocalMaxima_KernelConvolution**(*Data*, *framedim=(2048, 2048)*, *peakValConvolve=4*, *boxsizeConvolve=5*, *central_radiusConvolve=2*, *thresholdConvolve=1000*, *connectivity=1*, *IntensityThreshold=500*, *boxsize_for_probing_minimal_value_background=30*, *return_nb_raw_blobs=0*, *peakposition_definition='max'*)

return local maxima (blobs) position and amplitude in Data by using convolution with a mexican hat like kernel.

Two Thresholds are used sequently:

- thresholdConvolve : level under which intensity of kernel-convolved array is discarded
- IntensityThreshold : level under which blob whose local intensity amplitude in raw array is discarded

Parameters

Data : 2D array containing pixel intensities

peakValConvolve, boxsizeConvolve, central_radiusConvolve : convolution kernel parameters

thresholdConvolve [minimum threshold (expressed in unit of convolved array intensity)] under which convoluted blob is rejected.It can be zero (all blobs are accepted but time consuming)

connectivity [shape of connectivity pattern to consider pixels belonging to the]

same blob.

- 1: filled square (1 pixel connected to 8 neighbours)
- 0: star (4 neighbours in vertical and horizontal direction)

IntensityThreshold : minimum local blob amplitude to accept

boxsize_for_probing_minimal_value_background [boxsize to evaluate the background] and the blob amplitude

peakposition_definition [string ('max' or 'center')] key to assign to the blob position its hottest pixel position or its center (no weight)

Returns: –

peakslist [array like (n,2)] list of peaks position (pixel)

Ipixmax [array like (n,1) of integer] list of highest pixel intensity in the vicinity of each peak

npeaks [integer] nb of peaks (if return_nb_raw_blobs =1)

LaueTools.readmccd.**LocalMaxima_from_thresholdarray**(*Data*, *IntensityThreshold=400*, *rois=None*, *framedim=None*, *verbose=False*)

return center of mass of each blobs composes by pixels above IntensityThreshold

if Centers = list of (x,y, halfboxsizex, halfboxsizey) perform only blob search in theses ROIs

!warning!: center of mass of blob where all intensities are set to 1

LaueTools.readmccd.**localmaxima**(*DataArray*, *n*, *diags=1*, *verbose=0*)

from DataArray 2D returns (array([i1,i2,...,ip]),array([j1,j2,...,jp])) of indices where pixels value is higher in two direction up to n pixels

this tuple can be easily used after in the following manner: DataArray[tupleresult] is an array of the intensity of the hottest pixels in array

in similar way with only four cardinal directions neighbouring (found in the web): import numpy as N def local_minima(array2d):

return ((array2d <= np.roll(array2d, 1, 0)) & (array2d <= np.roll(array2d, -1, 0)) & (array2d <= np.roll(array2d, 1, 1)) & (array2d <= np.roll(array2d, -1, 1)))

WARNING: flat top peak are not detected !!

LaueTools.readmccd.**writepeaklist**(*tabpeaks*, *output_filename*, *outputfolder=None*, *comments=None*, *initialfilename=None*)

write peaks properties and comments in file with extension .dat added

LaueTools.readmccd.**fitoneimage_manypeaks**(*filename*, *peaklist*, *boxsize*, *stackimageindex=-1*, *CCDLabel='PRINCETON'*, *dirname=None*, *position_start='max'*, *type_of_function='gaussian'*, *guessed_peaksize=(1.0, 1.0)*, *xtol=0.001*, *FitPixelDev=2.0*, *Ipixmax=None*, *MaxIntensity=100000000000*, *MinIntensity=0*, *PeakSizeRange=(0, 200)*, *verbose=0*, *position_definition=1*, *NumberMaxofFits=500*, *ComputeIpixmax=False*, *use_data_corrected=None*, *reject_negative_baseline=True*, *purgeDuplicates=True*)

fit multiple ROI data to get peaks position in a single image

Ipixmax : highest intensity above background in every ROI centered on element of peaklist

use_data_corrected [enter data instead of reading data from file] must be a tuple of 3 elements: fulldata, framedim, fliprot where fulldata is an ndarray

purgeDuplicates : True remove duplicates that are close within pixel distance of 'boxsize' and keep the most intense peak

use_data_corrected [enter data instead of reading data from file] must be a tuple of 3 elements: fulldata, framedim, fliprot where fulldata ndarray

---

Note: used in PeakSearchGUI

LaueTools.readmccd.**PeakSearch**(*filename*, *stackimageindex=-1*, *CCDLabel='PRINCETON'*, *center=None*, *boxsizeROI=(200, 200)*, *PixelNearRadius=5*, *removeedge=2*, *IntensityThreshold=400*, *thresholdConvolve=200*, *paramsHat=(4, 5, 2)*, *boxsize=15*, *verbose=0*, *position_definition=1*, *local_maxima_search_method=1*, *peakposition_definition='max'*, *fit_peaks_gaussian=1*, *xtol=1e-05*, *return_histo=1*, *FitPixelDev=25*, *write_execution_time=1*, *Saturation_value=65535*, *Saturation_value_flatpeak=65535*, *MinIntensity=0*, *PeakSizeRange=(0, 200)*, *Data_for_localMaxima=None*, *Fit_with_Data_for_localMaxima=False*, *Remove_BlackListedPeaks_fromfile=None*, *maxPixelDistanceRejection=15.0*, *NumberMaxofFits=5000*, *reject_negative_baseline=True*, *formulaexpression='A-1.1*B'*, *listrois=None*)

Find local intensity maxima as starting position for fittinng and return peaklist.

Parameters filename : string

full path to image data file

stackimageindex [integer] index corresponding to the position of image data on a stacked images file if -1 means single image data w/o stacking

CCDLabel [string] label for CCD 2D detector used to read the image data file see dict_LaueTools.py

center : position #TODO: to be removed: position of the ROI center in CCD frame

boxsizeROI [dimensions of the ROI to crop the data array] only used if center != None

boxsize [half length of the selected ROI array centered on each peak:] for fitting a peak for estimating the background around a peak for shifting array in second method of local maxima search (shifted arrays)

IntensityThreshold [integer]

pixel intensity level above which potential peaks are kept for fitting position procedure

for local maxima method 0 and 1, this level is relative to zero intensity for local maxima method 2, this level is relative to lowest intensity in the ROI (local background) start with high value If too high, few peaks are found (only the most important) If too low, too many local maxima are found leading to time consuming fitting procedure

thresholdConvolve [integer] pixel intensity level in convolved image above which potential peaks are kept for fitting position procedure This threshold step on convolved image is applied prior to the local threshold step with IntensityThreshold on initial image (with respect to the local background)

paramsHat : mexican hat kernel parameters (see `LocalMaxima_ndimage()`)

PixelNearRadius: integer

pixel distance between two regions considered as peaks

start rather with a large value. If too low, there are very much peaks duplicates and this is very time consuming

local_maxima_search_method [integer]

Select method for find the local maxima, each of them will fitted

: 0 extract all pixel above intensity threshold : 1 find pixels are highest than their neighbours in horizontal, vertical

and diagonal direction (up to a given pixel distance)

: 2 find local hot pixels which after numerical convolution give high intensity above threshold (thresholdConvolve) then threshold (IntensityThreshold) on raw data

peakposition_definition ['max' or 'center' for local_maxima_search_method == 2]

to assign to the blob position its hottest pixel position or its center (no weight)

Saturation_value_flatpeak : saturation value of detector for local maxima search method 1

Remove_BlackListedPeaks_fromfile [None or full file path to a peaklist file containing peaks] that will be deleted in peak list resulting from the local maxima search procedure (prior to peak refinement)

maxPixelDistanceRejection [maximum distance between black listed peaks and current peaks] (found by peak search) to be rejected

NumberMaxofFits : highest acceptable number of local maxima peak to be refined with a 2D modelPeakSearch

fit_peaks_gaussian [0 no position and shape refinement procedure performed from local maxima (or blob) results] : 1 2D gaussian peak refinement : 2 2D lorentzian peak refinement

xtol : relative error on solution (x vector) see args for leastsq in scipy.optimize FitPixelDev : largest pixel distance between initial (from local maxima search)

and refined peak position

position_definition: due to various conventional habits when reading array, add some offset to fitdata XMAS or fit2d peak = 0 no offset (python numpy convention) = 1 XMAS offset = 2 fit2d offset

return_histo [0 3 output elements] : 1 4 elemts, last one is histogram of data : 2 4 elemts, last one is the nb of raw blob found after convolution and threshold

Data_for_localMaxima [object to be used only for initial step of finding local maxima (blobs) search]

(and not necessarly for peaks fitting procedure):

- ndarray = array data
- 'auto_background' = calculate and remove background computed from image data itself (read in file 'filename')
- path to image file (string) = B image to be used in a mathematical operation with Ato current image

Fit_with_Data_for_localMaxima [use 'Data_for_localMaxima' object as image when refining peaks position and shape] with initial peak position guess from local maxima search

formulaexpression [string containing A (raw data array image) and B (other data array image)] expressing mathematical operation,e.g: 'A-3.2*B+10000' for simple background substraction (with B as background data): 'A-B' or 'A-alpha*B' with alpha > 1.

reject_negative_baseline [True reject refined peak result if intensity baseline (local background) is negative] (2D model is maybe not suitable)

returns:

peak list sorted by decreasing (integrated intensity - fitted bkg) peak_X,peak_Y,peak_I,peak_fwaxmaj,peak_fwaxmin,peak_inclina

for fit_peaks_gaussian == 0 (no fitdata) and local_maxima_search_method==2 (convolution) if peakposition_definition ='max' then X,Y,I are from the hottest pixels if peakposition_definition ='center' then X,Y are blob center and I the hottest blob pixel

nb of output elements depends on 'return_histo' argument

LaueTools.readmccd.**peaksearch_on_Image**(*filename_in*, *pspfile*, *background_flag='no'*, *blacklistpeaklist=None*, *dictPeakSearch={}*, *CCDLabel='MARCCD165'*, *outputfilename=None*, *psdict_Convolve={'Data_for_localMaxima': 'auto_background', 'FitPixelDev': 2.0, 'IntensityThreshold': 10, 'NumberMaxofFits': 5000, 'PixelNearRadius': 10, 'boxsize': 15, 'fit_peaks_gaussian': 1, 'local_maxima_search_method': 2, 'position_definition': 1, 'removeedge': 2, 'return_histo': 0, 'thresholdConvolve': 500, 'verbose': 0, 'write_execution_time': 0, 'xtol': 0.001}*)

Perform a peaksearch by using .psp file

still not very used and checked? # missing dictPeakSearch as function argument for formulaexpression or dict_param??

LaueTools.readmccd.**read_background_flag**(*background_flag*)
interpret the background flag (field used in FileSeries/Peak_Search.py)

return two values to put in dict_param of peaksearch_series

LaueTools.readmccd.**plot_image_markers**(*image*, *markerpos*, *position_definition=1*)
plot 2D array (image) with markers at first two columns of (markerpos)

Note: used in LaueHDF5. Could be better implementation in some notebooks

---

LaueTools.readmccd.**applyformula_on_images**(*A*, *B*, *formulaexpression='A-B'*, *SaturationLevel=None*, *clipintensities=True*)

calculate image data array from math expression

A, B : ndarray of the same shape

SaturationLevel : saturation level of intensity

clipintensities : clip resulting intensities to zero and saturation value

LaueTools.readmccd.**peaksearch_fileseries**(*fileindexrange*, *filenameprefix*, *suffix=''*, *nbdigits=4*, *dirname_in='/home/micha/LaueProjects/AxelUO2'*, *outputname=None*, *dirname_out=None*, *CCDLABEL='MARCCD165'*, *KF_DIRECTION='Z>0'*, *dictPeakSearch=None*)

peaksearch function to be called for multi or single processing

LaueTools.readmccd.**peaksearch_multiprocessing**(*fileindexrange*, *filenameprefix*, *suffix=''*, *nbdigits=4*, *dirname_in='/home/micha/LaueProjects/AxelUO2'*, *outputname=None*, *dirname_out=None*, *CCDLABEL='MARCCD165'*, *KF_DIRECTION='Z>0'*, *dictPeakSearch=None*, *nb_of_cpu=2*)

launch several processes in parallel

LaueTools.readmccd.**gauss_kern**(*size*, *sizey=None*)
Returns a normalized 2D gauss kernel array for convolutions

LaueTools.readmccd.**blur_image**(*im*, *n*, *ny=None*)

blurs the image by convolving with a gaussian kernel of typical size n. The optional keyword argument ny allows for a different size in the y direction.

LaueTools.readmccd.**blurCCD**(*im*, *n*)
apply a blur filter to image ndarray

LaueTools.readmccd.**circularMask**(*center*, *radius*, *arrayshape*)
return a boolean ndarray of elem in array inside a mask

LaueTools.readmccd.**compute_autobackground_image**(*dataimage*, *boxsizefilter=10*)
return 2D array of filtered data array :param dataimage: array of image data :type dataimage: 2D array

LaueTools.readmccd.**computefilteredimage**(*dataimage*, *bkg_image*, *CCDlabel*, *kernelsize=5*, *formulaexpression='A-B'*, *usemask=True*)
return 2D array of initial image data without background given by bkg_image data

usemask [True then substract bkg image on masked raw data] False apply formula on all pixels (no mask)

Parameters

- **dataimage** (*2D array*) – array of image data
- **bkg_image** (*2D array*) – array of filtered image data (background)
- **CCDlabel** (*string*) – key for CCD dictionary

LaueTools.readmccd.**filterimage**(*image_array*, *framedim*, *blurredimage=None*, *kernelsize=5*, *mask_parameters=None*, *clipvalues=None*, *imageformat=<class 'numpy.uint16'>*)
compute a difference of images inside a region defined by a mask

blurredimage: ndarray image to substract to image_array kernelsize: pixel size of gaussian kernel if blurredimage is None

mask_parameters: circular mask parameter: center=(x,y), radius, value outside mask

LaueTools.readmccd.**blurCCD_with_binning**(*im*, *n*, *binsize=(2, 2)*)
blur the array by rebinning before and after aplying the filter

LaueTools.readmccd.**remove_minimum_background**(*im*, *boxsize=10*)
remove to image array the array resulting from minimum_filter

LaueTools.readmccd.**purgePeaksListFile**(*filename1*, *blacklisted_XY*, *dist_tolerance=0.5*, *dirname=None*)
remove in peaklist .dat file peaks that are in blacklist

blacklisted_XY: [X1,Y1],[X2,Y2]

LaueTools.readmccd.**write_PurgedPeakListFile**(*filename1*, *blacklisted_XY*, *outputfilename*, *dist_tolerance=0.5*, *dirname=None*)
write a new .dat file where peaks in blacklist are omitted

LaueTools.readmccd.**removePeaks_inPeakList**(*PeakListfilename*, *BlackListed_PeakListfilename*, *outputfilename*, *dist_tolerance=0.5*, *dirname=None*)
read peaks PeakListfilename and remove those in BlackListed_PeakListfilename and write a new peak list file

---

Note: Not used ??

LaueTools.readmccd.**merge_2Peaklist**(*filename1*, *filename2*, *dist_tolerance=5*, *dirname1=None*, *dirname2=None*, *verbose=0*)
return merge spots data from two peaklists and removed duplicates within dist_tolerance (pixel)

LaueTools.readmccd.**writefile_mergedPeaklist**(*filename1*, *filename2*, *outputfilename*, *dist_tolerance=5*, *dirname1=None*, *dirname2=None*, *verbose=0*)

write peaklist file from the merge of spots data from two peaklists (and removed duplicates within dist_tolerance (pixel))

7.4 Modules for Laue Pattern Indexation

7.5 Modules for Crystal unit cell refinement

7.6 Modules for batch processing

PYTHON MODULE INDEX

l

LaueTools.CrystalParameters, 53
LaueTools.GUI.PeakSearchGUI, 86
LaueTools.lauecore, 59
LaueTools.LaueGeometry, 69
LaueTools.multigrainsSimulator, 75
LaueTools.readmccd, 91

INDEX

A

activateCrop() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
Add_Images() (in module LaueTools.readmccd), 95
AngleBetweenNormals() (in module LaueTools.CrystalParameters), 57
applyformula_on_images() (in module LaueTools.readmccd), 101
askUserForDirname() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 88

B

bestposition() (LaueTools.GUI.PeakSearchGUI.ViewColorPanel method), 87
blur_image() (in module LaueTools.readmccd), 101
blurCCD() (in module LaueTools.readmccd), 102
blurCCD_with_binning() (in module LaueTools.readmccd), 102
BrowseCropPanel (class in LaueTools.GUI.PeakSearchGUI), 87
buildMosaic() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90

C

calc_B_RR() (in module LaueTools.CrystalParameters), 57
calc_uflab() (in module LaueTools.LaueGeometry), 70
calc_uflab_trans() (in module LaueTools.LaueGeometry), 71
calc_xycam() (in module LaueTools.LaueGeometry), 71
calc_xycam_transmission() (in module LaueTools.LaueGeometry), 71
calcSpots_fromHKLlist() (in module LaueTools.lauecore), 63
check_array_indices() (in module LaueTools.readmccd), 95
circularMask() (in module LaueTools.readmccd), 102
compute_autobackground_image() (in module LaueTools.readmccd), 102
Compute_data2thetachi() (in module LaueTools.LaueGeometry), 73
computefilteredimage() (in module LaueTools.readmccd), 102
Computefilteredimage() (LaueTools.GUI.PeakSearchGUI.FilterBackGroundPanel method), 87
Construct_GrainsParameters_parametric() (in module LaueTools.multigrainsSimulator), 75
convert2corfile() (in module LaueTools.LaueGeometry), 73
convert2corfile_fileseries() (in module LaueTools.LaueGeometry), 74
convert2corfile_multiprocessing() (in module LaueTools.LaueGeometry), 74
convert_xycam_from_sourceshift() (in module LaueTools.LaueGeometry), 74
ConvolvebyKernel() (in module LaueTools.readmccd), 97
create_main_panel() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 88
create_spot() (in module LaueTools.lauecore), 61
create_spot_np() (in module LaueTools.lauecore), 61
CurrentFileIsReady() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89

D

deleteAllPeaks() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 91
deleteOnePeak() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 91
DeviatoricStrain_LatticeParams() (in module LaueTools.CrystalParameters), 58
diff_pix() (in module LaueTools.readmccd), 95
dosimulation_parametric() (in module LaueTools.multigrainsSimulator), 75
draw_cursor() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90

F

FilterBackGroundPanel (class in LaueTools.GUI.PeakSearchGUI), 87

Tools.GUI.PeakSearchGUI), 87
FilterHarmonics_2() (in module LaueTools.CrystalParameters), 57
filterimage() (in module LaueTools.readmccd), 102
filterLaueSpots() (in module LaueTools.lauecore), 61
findLocalMaxima_Meth_1 (class in LaueTools.GUI.PeakSearchGUI), 88
findLocalMaxima_Meth_2 (class in LaueTools.GUI.PeakSearchGUI), 88
findLocalMaxima_Meth_3 (class in LaueTools.GUI.PeakSearchGUI), 88
fitoneimage_manypeaks() (in module LaueTools.readmccd), 98
FitParametersPanel (class in LaueTools.GUI.PeakSearchGUI), 88
from_qunit_to_twchi() (in module LaueTools.LaueGeometry), 72
from_twchi_to_q() (in module LaueTools.LaueGeometry), 72
from_twchi_to_qunit() (in module LaueTools.LaueGeometry), 72

G

gauss_kern() (in module LaueTools.readmccd), 101
genHKL_np() (in module LaueTools.lauecore), 59
get2ThetaChi_geometry() (in module LaueTools.lauecore), 62
Get_XYI_from_fit2dpeaksfile() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
getclickposition() (LaueTools.GUI.PeakSearchGUI.ViewColorPanel method), 86
getClosestPeak() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 91
getConvolvedData() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
getDisplayedImageSize() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
getExtrema() (in module LaueTools.readmccd), 96
getIndex_fromfilename() (in module LaueTools.readmccd), 91
getIndex_fromfilename() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
getindices2cropArray() (in module LaueTools.readmccd), 94
getIntegratedIntensities() (in module LaueTools.readmccd), 96
getIntegratedIntensity() (in module LaueTools.readmccd), 96
getLaueSpots() (in module LaueTools.lauecore), 60
getlineprofiledata() (LaueTools.GUI.PeakSearchGUI.PlotPeakListPanel method), 88
getlineprofiledata() (LaueTools.GUI.PeakSearchGUI.ViewColorPanel method), 87
getMinMax() (in module LaueTools.readmccd), 96
gettime() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
GrainParameter_from_Material() (in module LaueTools.CrystalParameters), 53

I

init_figure_draw() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89

L

LaueTools.CrystalParameters (module), 53
LaueTools.GUI.PeakSearchGUI (module), 86
LaueTools.lauecore (module), 59
LaueTools.LaueGeometry (module), 69
LaueTools.multigrainsSimulator (module), 75
LaueTools.readmccd (module), 91
lengthInSample() (in module LaueTools.LaueGeometry), 74
line_select_callback() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 88
localmaxima() (in module LaueTools.readmccd), 98
LocalMaxima_from_thresholdarray() (in module LaueTools.readmccd), 97
LocalMaxima_KernelConvolution() (in module LaueTools.readmccd), 97
LoGArr() (in module LaueTools.readmccd), 96

M

MainPeakSearchFrame (class in LaueTools.GUI.PeakSearchGUI), 88
matrix_to_rlat() (in module LaueTools.CrystalParameters), 59
merge_2Peaklist() (in module LaueTools.readmccd), 102
MosaicAndMonitor (class in LaueTools.GUI.PeakSearchGUI), 87

N

normalizeplot() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90

O

onCenterROI() (LaueTools.GUI.PeakSearchGUI.ROISelection method), 87

onChangeIndex_slider_imagevert() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
OnChangeUseFormula() (LaueTools.GUI.PeakSearchGUI.FilterBackGroundPanel method), 87
OnCheckPlotValues() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
onClick() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 88
onComputeBlurImage() (LaueTools.GUI.PeakSearchGUI.FilterBackGroundPanel method), 87
OnFit() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
onFitOnePeak() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
onGetBImagefilename() (LaueTools.GUI.PeakSearchGUI.FilterBackGroundPanel method), 87
onGetBlackListfilename() (LaueTools.GUI.PeakSearchGUI.FilterBackGroundPanel method), 87
OnGoto() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
onKeyPressed() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
OnLargeMinus() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
OnLargePlus() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
OnMinus() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
OnMosaic() (LaueTools.GUI.PeakSearchGUI.MosaicAndMonitor method), 87
onMotion_ToolTip() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
onOpenDetFile() (LaueTools.GUI.PeakSearchGUI.ViewColorPanel method), 87
OnPeakSearch() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 91
OnPlus() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
OnRemove() (LaueTools.GUI.PeakSearchGUI.PeakListOLV method), 88
onRemoveAllPeakstoPeaklist() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
onRemovePeaktoPeaklist() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
OnReplot() (LaueTools.GUI.PeakSearchGUI.ViewColorPanel method), 86
onSaveBlurImage() (LaueTools.GUI.PeakSearchGUI.FilterBackGroundPanel method), 87
onSaveFormulaResultImage() (LaueTools.GUI.PeakSearchGUI.FilterBackGroundPanel method), 87
onSaveROIsList() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
OnSetFileCCDParam() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 88
OnSetPlotSize() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 88
OnShowLineProfiler() (LaueTools.GUI.PeakSearchGUI.PlotPeakListPanel method), 88
OnShowLineProfiler() (LaueTools.GUI.PeakSearchGUI.ViewColorPanel method), 87
OnShowLineXYProfiler() (LaueTools.GUI.PeakSearchGUI.PlotPeakListPanel method), 88
OnShowLineXYProfiler() (LaueTools.GUI.PeakSearchGUI.ViewColorPanel method), 86
OnSpinCtrl_ImaxDisplayed() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
OnSwitchBlurRawImage() (LaueTools.GUI.PeakSearchGUI.FilterBackGroundPanel method), 87
OnSwitchImageDisplay() (LaueTools.GUI.PeakSearchGUI.findLocalMaxima_Meth_3 method), 88
OnTabChange_nb0() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 88
onToggle() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
onToggleCrop() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89

P

PeakListOLV (class in LaueTools.GUI.PeakSearchGUI), 88
PeakSearch() (in module LaueTools.readmccd), 98

peaksearch_fileseries() (in module LaueTools.readmccd), 101
peaksearch_multiprocessing() (in module LaueTools.readmccd), 101
peaksearch_on_Image() (in module LaueTools.readmccd), 100
plot_image_markers() (in module LaueTools.readmccd), 101
PlotPeakListPanel (class in LaueTools.GUI.PeakSearchGUI), 88
PlotValues() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
Prepare_Grain() (in module LaueTools.CrystalParameters), 55
purgePeaksListFile() (in module LaueTools.readmccd), 102

Q

Quicklist() (in module LaueTools.lauecore), 59
qvector_from_xy_E() (in module LaueTools.LaueGeometry), 72

R

read_background_flag() (in module LaueTools.readmccd), 101
read_data() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
Read_GrainListparameter() (in module LaueTools.multigrainsSimulator), 75
read_header_marccd() (in module LaueTools.readmccd), 91
read_header_marccd2() (in module LaueTools.readmccd), 91
read_header_scmos() (in module LaueTools.readmccd), 92
readCCDimage() (in module LaueTools.readmccd), 92
readdata_updateplot_aftercrop_uncrop() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
readheader() (in module LaueTools.readmccd), 91
readoneimage() (in module LaueTools.readmccd), 92
readoneimage_crop() (in module LaueTools.readmccd), 93
readoneimage_crop_fast() (in module LaueTools.readmccd), 92
readoneimage_manycrops() (in module LaueTools.readmccd), 93
readoneimage_multiROIfit() (in module LaueTools.readmccd), 93
readrectangle_in_image() (in module LaueTools.readmccd), 93
reinit_aftercrop_draw() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
remove_minimum_background() (in module LaueTools.readmccd), 102
removePeaks_inPeakList() (in module LaueTools.readmccd), 102
restrictxylimits_to_imagearray() (LaueTools.GUI.PeakSearchGUI.ViewColorPanel method), 87
ROISelection (class in LaueTools.GUI.PeakSearchGUI), 87

S

SavePeakList_PSPfile() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
set_circleradius() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
setfilename() (in module LaueTools.readmccd), 91
setfilename() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
Show_ConvolvedImage() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
Show_Image() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
showImage() (LaueTools.GUI.PeakSearchGUI.ViewColorPanel method), 87
SimulateLaue() (in module LaueTools.lauecore), 63
SimulateLaue_full_np() (in module LaueTools.lauecore), 65
SimulateResult() (in module LaueTools.lauecore), 67
SumImages() (in module LaueTools.readmccd), 95

T

to8bits() (in module LaueTools.readmccd), 95
toplayout2() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 88

U

uflab_from2thetachi() (in module LaueTools.LaueGeometry), 71
unit_q() (in module LaueTools.LaueGeometry), 73
update() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 89
update_draw() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90
updateLineXYProfile() (LaueTools.GUI.PeakSearchGUI.ViewColorPanel method), 87
updatePlotTitle() (LaueTools.GUI.PeakSearchGUI.MainPeakSearchFrame method), 90

V

vec_normalTosurface() (in module LaueTools.LaueGeometry), 74
vec_onsurface_alongys() (in module LaueTools.LaueGeometry), 74
ViewColorPanel (class in LaueTools.GUI.PeakSearchGUI), 86
VolumeCell() (in module LaueTools.CrystalParameters), 58, 59

W

write_PurgedPeakListFile() (in module LaueTools.readmccd), 102
write_rawbinary() (in module LaueTools.readmccd), 95
writefile_mergedPeaklist() (in module LaueTools.readmccd), 102
writeimage() (in module LaueTools.readmccd), 95
writepeaklist() (in module LaueTools.readmccd), 98