
LaueTools

A software package for Laue microdiffraction data analysis

<https://sourceforge.net/projects/lauetools/>

Jean Sébastien MICHA

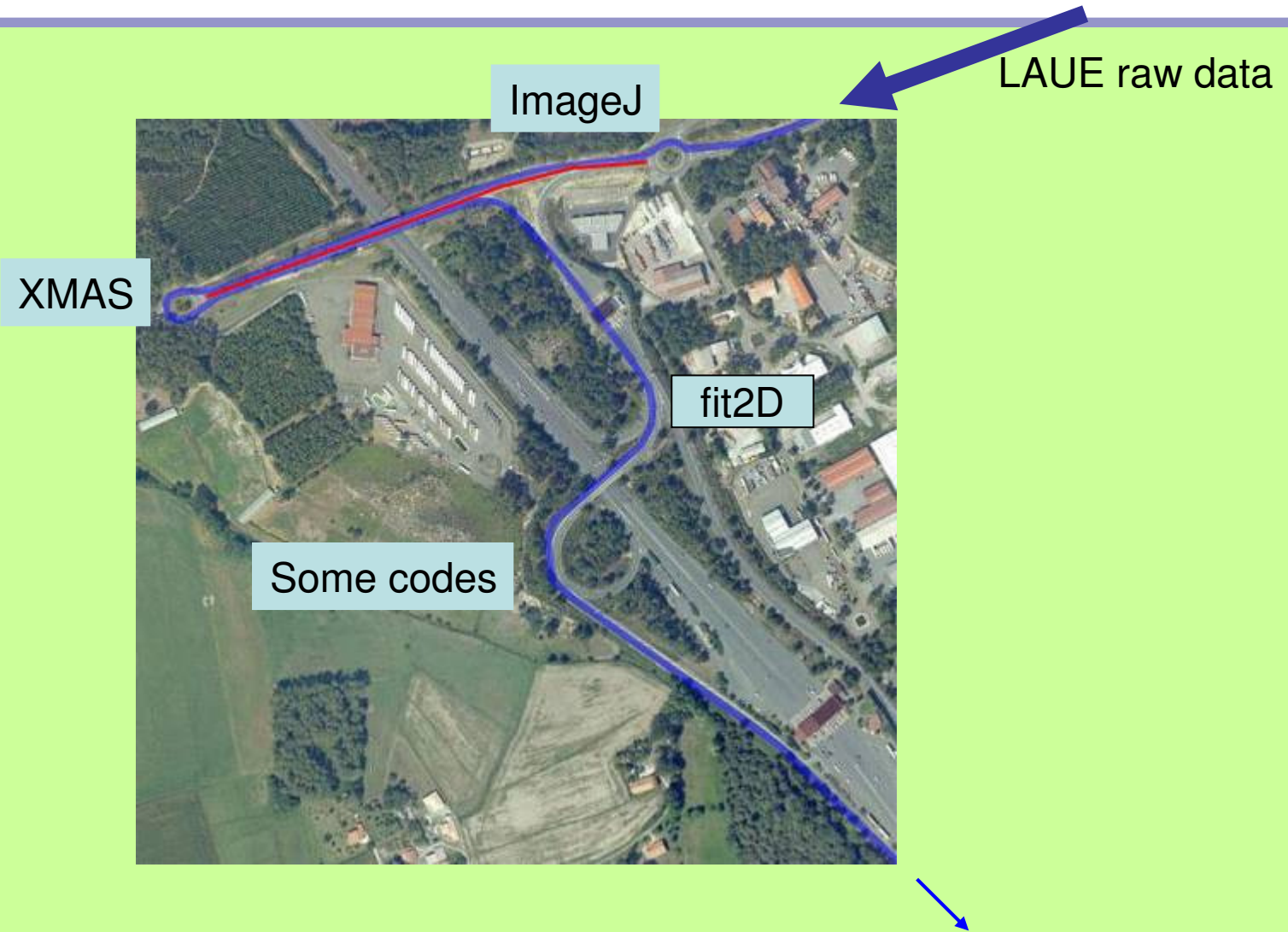
UMR SPRAM CNRS-Grenoble & CRG-IF BM32 at ESRF

25th September 2009

Motivations



Motivations



Motivations



LAUE raw data

LaueTools

makes data flow easier ...

Motivations

Fast data acquisition rate But slow analysis rate

X-ray Microdiffraction Analysis Software (XMAS) by N. Tamura

GREAT but:

- *Black box*
- *Poorly documented*
- *Low intermediate user input*
- *No new functionalities*
- *No bashable*

Lauetools is for increasing scientific throughput of μ Laue

- *online/offline analysis*
- *help on data acquisition strategy*
- *GUI, command line, bashable*
- *open-source:*
 - *stimulate development and maintenance*
 - *user control of codes and models*
 - *interactions between mechanics, physics, Xtallographers, programmer...*

Motivations

Codes in python

OO, script, easy prototyping

open-source

multi-platform

matlab-like libraries:

 matplotlib

 numpy

stats, optimisation

graph, bayes

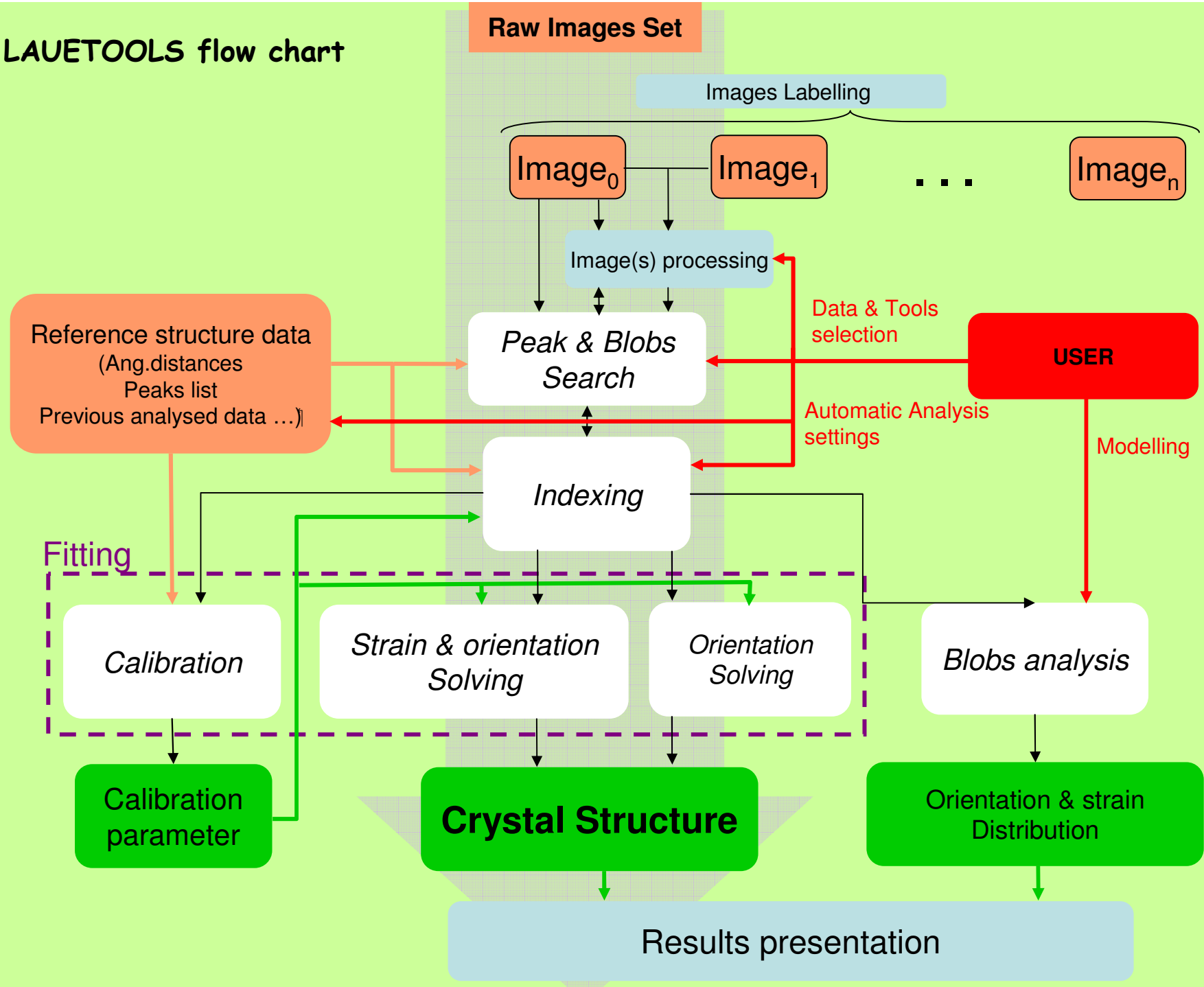
wxpython

Modularity, Separated routines, classes

Interactive python

interface with C, JAVA, Fortran

LAUETOOLS flow chart



LAUETOOLS implementation

GUI in wxpython

LaueTool.py

Visualisation
Indexing
Structure
refinement
Results
visualisation

3D visualisation in PyOpenGL

laue3D.py

Data representation
Quick U estimation
Strain & Energy effect

readmccd.py

image data reading
digital processing, numerical operations

fit2dintensity.py

2D intensity profile fitting

gnomon.py

projection on to gnomonic plane
Hough transform
data and reference matching

laue.py

Laue pattern simulation

findorient.py

orientation matrix U determination

calibrate.py
geometry calibration

detector and experiment
camera vision + minimisation process

calcdef.py

Strain determination (B matrix)

graingraph.py

cliques finding

find2thetachi.py

coordinates transforms

recognition.py

spot and zone recognition

LAUETOOLS' world

Image

Binary data ~ TIFF+header
prefix_####.ext
prefix_####

####: 4 digits integer number
Ext: mccd, tiff, spe

IMAGE PROCESSING

LAUETOOL
PIL

ImageJ plugins

PEAK SEARCH

FIT2D
Batch, Python subprocess

LAUETOOL

XMAS
(indexation dependent)

ImageJ plugin

Peaks list

Ascii multicolumns data file
prefix_####.ext

Ext: peaks,pic,...

CALIBRATION

LAUETOOL
XMAS

Peaks list

Ascii multiicolumns data file
prefix_####.cor

INDEXATION

LAUETOOL

automatic

manual

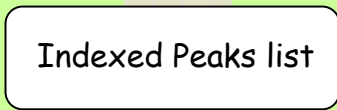
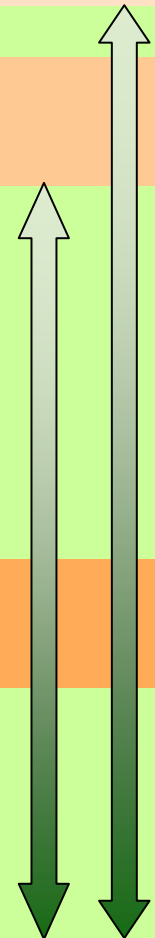
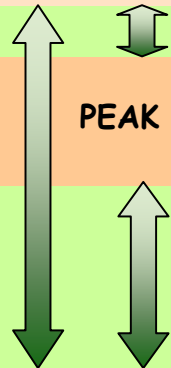
computer-aided

Indexed Peaks list

Ascii multiicolumns data file
prefix_####.ind

STRUCTURE REFINEMENT

LAUETOOL



LAUETOOLS current status

◆ Simulation

➤➤ General and pedagogical tool (laue3D)

Input:

➤➤ Detector geometry: transmission, backreflection, side, top

➤➤ Spectral Range

Materials parameters

➤➤ multigrains

➤➤ orientation matrix (U)

➤➤ lattice matrix (B)

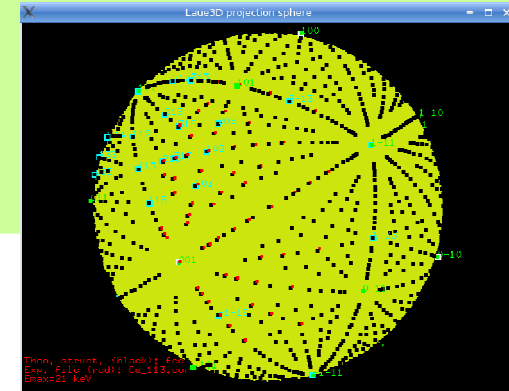
➤➤ some transforms on U,B: twins, mosaicity, strain gradient

Output:

➤➤ Ascii file

➤➤ Spot objects list

➤➤ Plot



LAUETOOLS current status

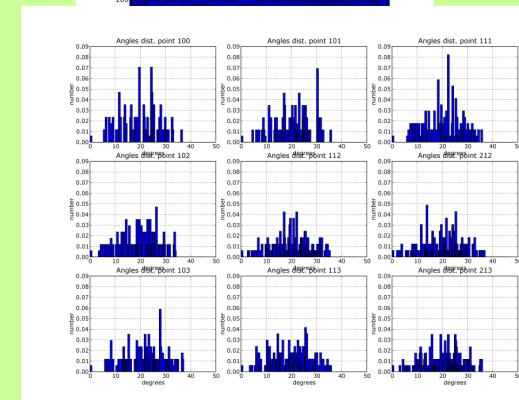
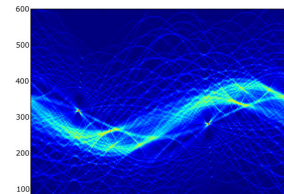
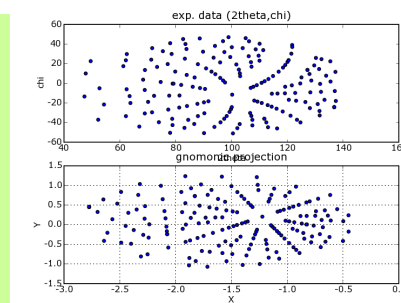
- ◆ Simulation
- ◆ Data pre-processing

- Basic Grain mapping (most intense peak)
- Peak search (basic, digital processing)

◆ Indexing

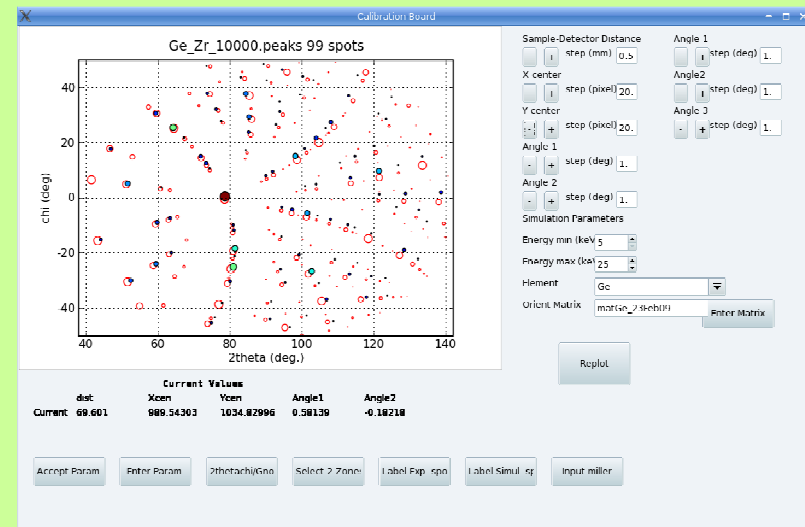
- manual -> automatic
- brute force (trials and errors)
- image comparing (in Hough space) (~ no peak search)
- information selection (Human-computer collaboration)

gnomonic projection
hough space
cliques
spot & zone axis recognition



LAUETOOLS current status

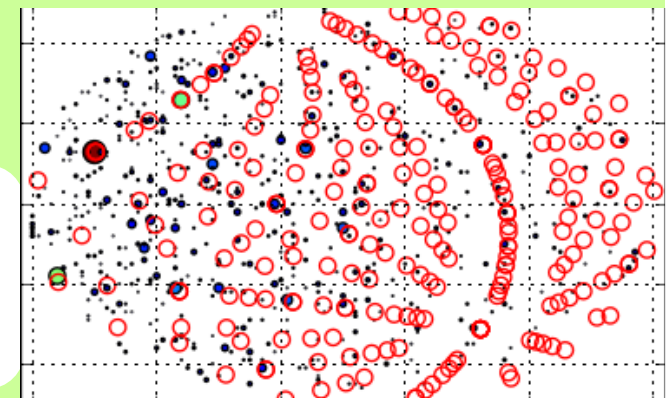
- ◆ Simulation
- ◆ Data pre-processing
- ◆ Indexing
- ◆ Structure solving



- Detector calibration: refinement, camera & perspective vision
- Strain Refinement

◆ Visualisation

- Data representation & manual indexing
- Graphical User Interface: data visualisation & indexing
- Only ideas and trials for results visualisation



LAUETOOLS perspectives

- Automatic indexing & structure refinement of file series
- Documentation
- Autonomy in pre-processing

- Open-source dev, cvs, executables distribution
- Workshop on « microLaue Diffraction and analysis »

- More physics & Xtallography & metallurgy models input
- Quantifying experts performance and scopes
- More experts for indexing

- Parallel computing
- ...



Upcoming techniques

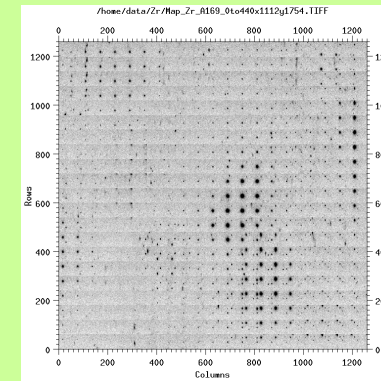
- 3D microLaue Diffraction
- Laue spot tomography
- intensity harvesting

Interactions with TotalCryst & Fable (algorithms & Laue plugins)

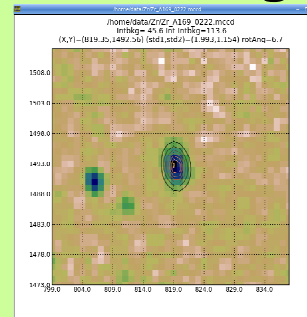
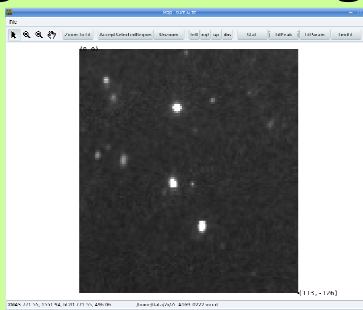
Extension of image viewer and other tools:
Images slicing, plot vs exp. Conditions
statistics and geometrical maths

Data analysis and visualisation tools

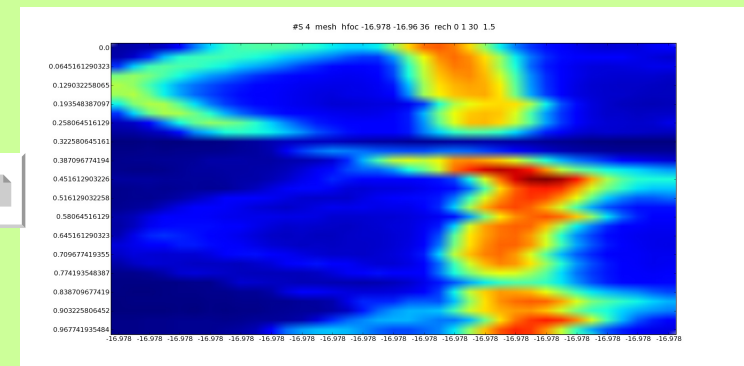
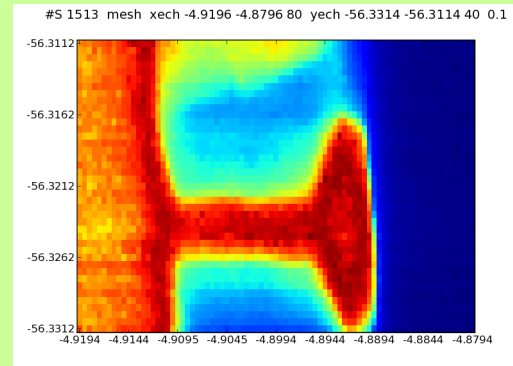
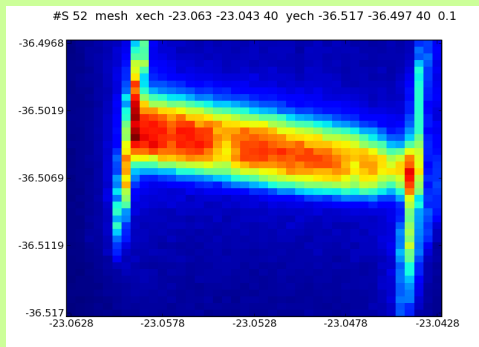
- ◆ mosaic



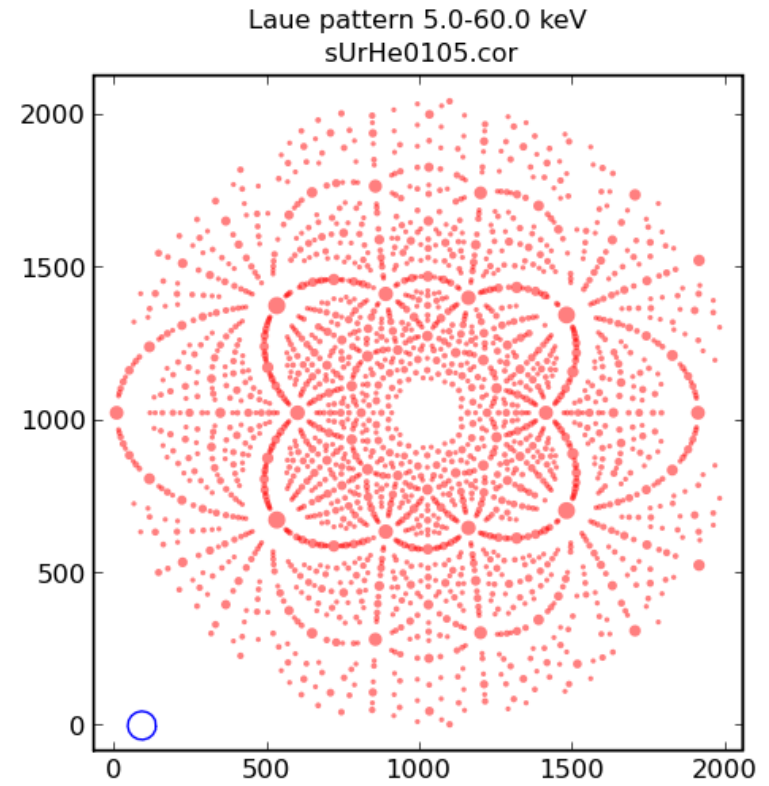
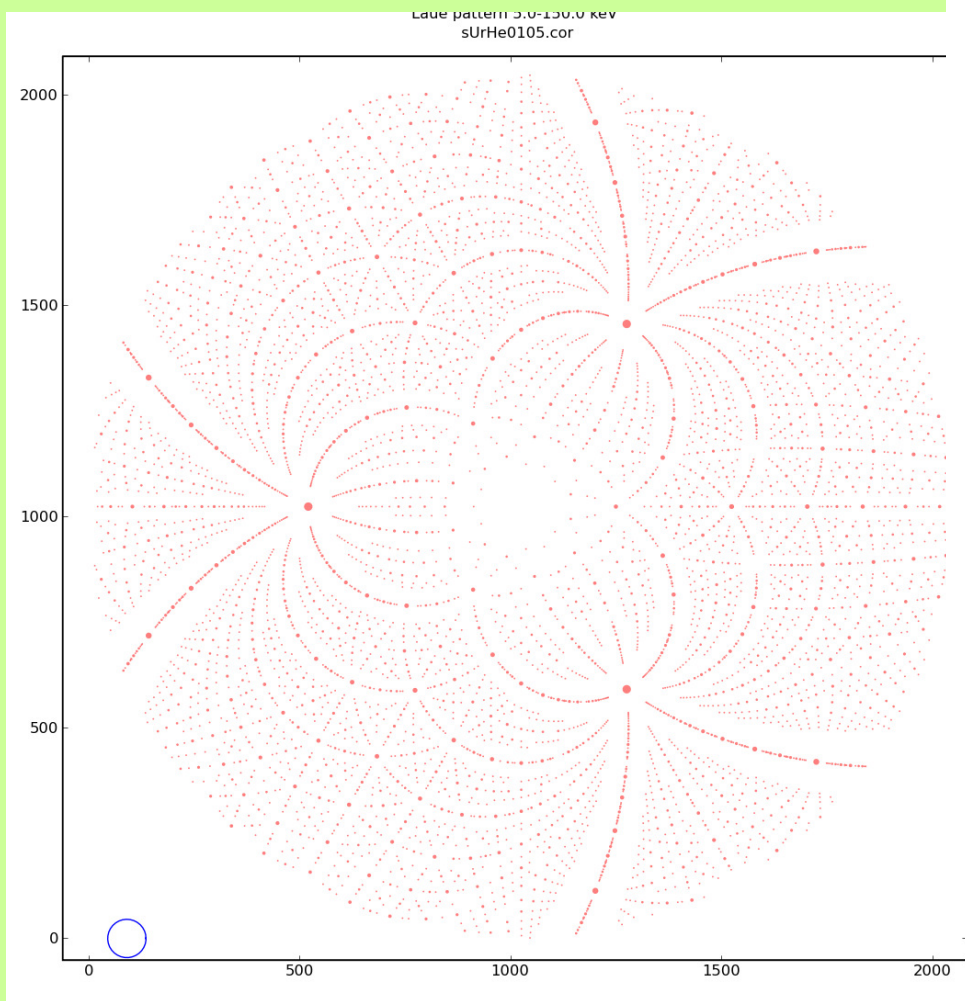
- ◆ Images set navigator & processing



- ◆ plotmesh



Transmission



Back-reflection



Element: a*,b*,c*: Rot. Matrix: Strain:

Grain Name	Element	a*,b*,c*	Rot. Matrix	Strain	Transform
Grain_0	Cu	Default	Identity	Unstrained	
Grain_1	Cu	Default	Identity	Unstrained	Tt_0

Transformations (MicroStrain and MisOrientation)

ROTATION

No rotation varying
 Axis-angle Variation (a: absolute,s:sample)
 Axis:
 Angle (deg):
 Element matrix

STRAIN

No strain varying
 Axis-traction (a: absolute,s:sample,c:crys)
 Axis 1 s[0,0,1] fact:
 Axis 2 s[1,1,0] fact:
 Axis 3 c[1,1,1] fact:
 Element matrix (a: absolute,s:sample,c:crys)

Spectral Band (keV)


Energy min:
 Energy max:

Plot Parameters

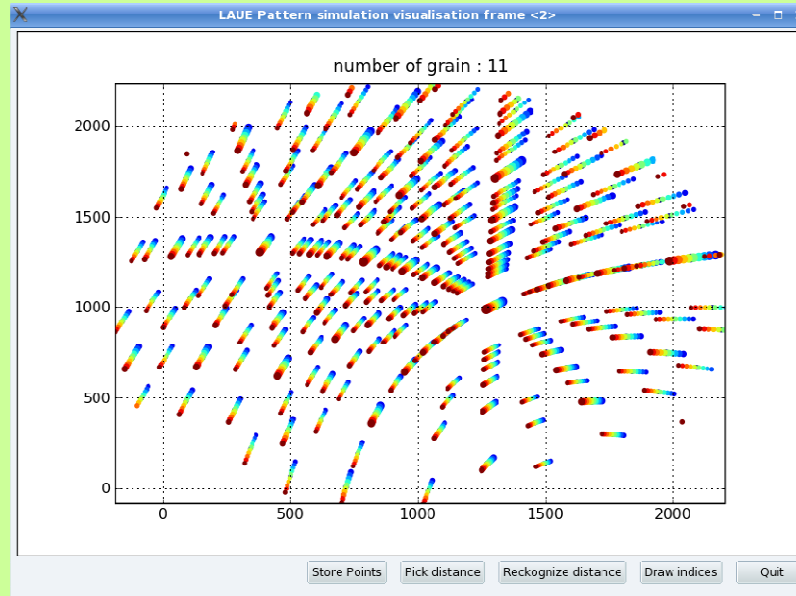
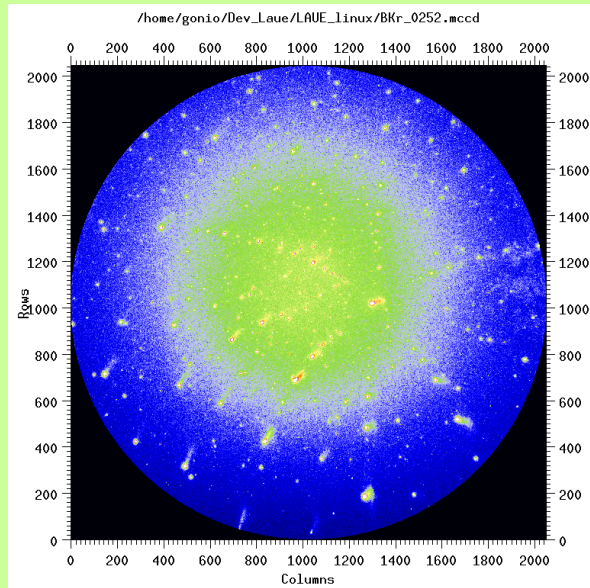
Show Plot Det. Dist. (mm):
 Camera on top Det. Diam. (mm):
 Camera on side +xcen (pix):
 Camera on side - ycen (pix):
 2ThetaChi XYmar XYfit2d

File Parameters

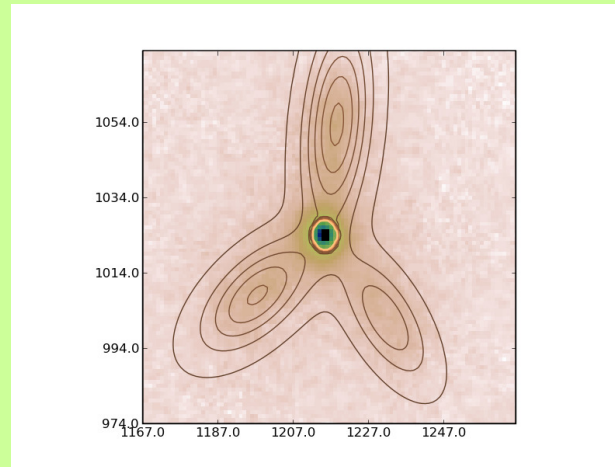
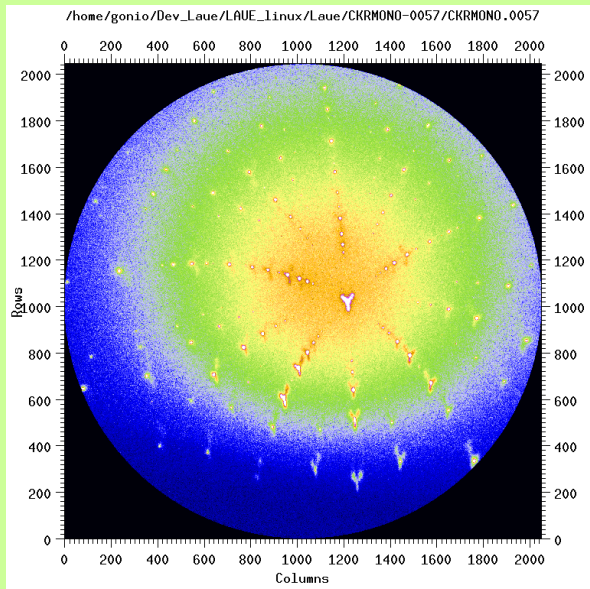
Directory:
 Save File
 Manual myfilename .sim
 Auto. Indexed mySimul_ .sim
 Create .cor f mySimul_ .cor

Laue Simulation Completed






Slip system activated !



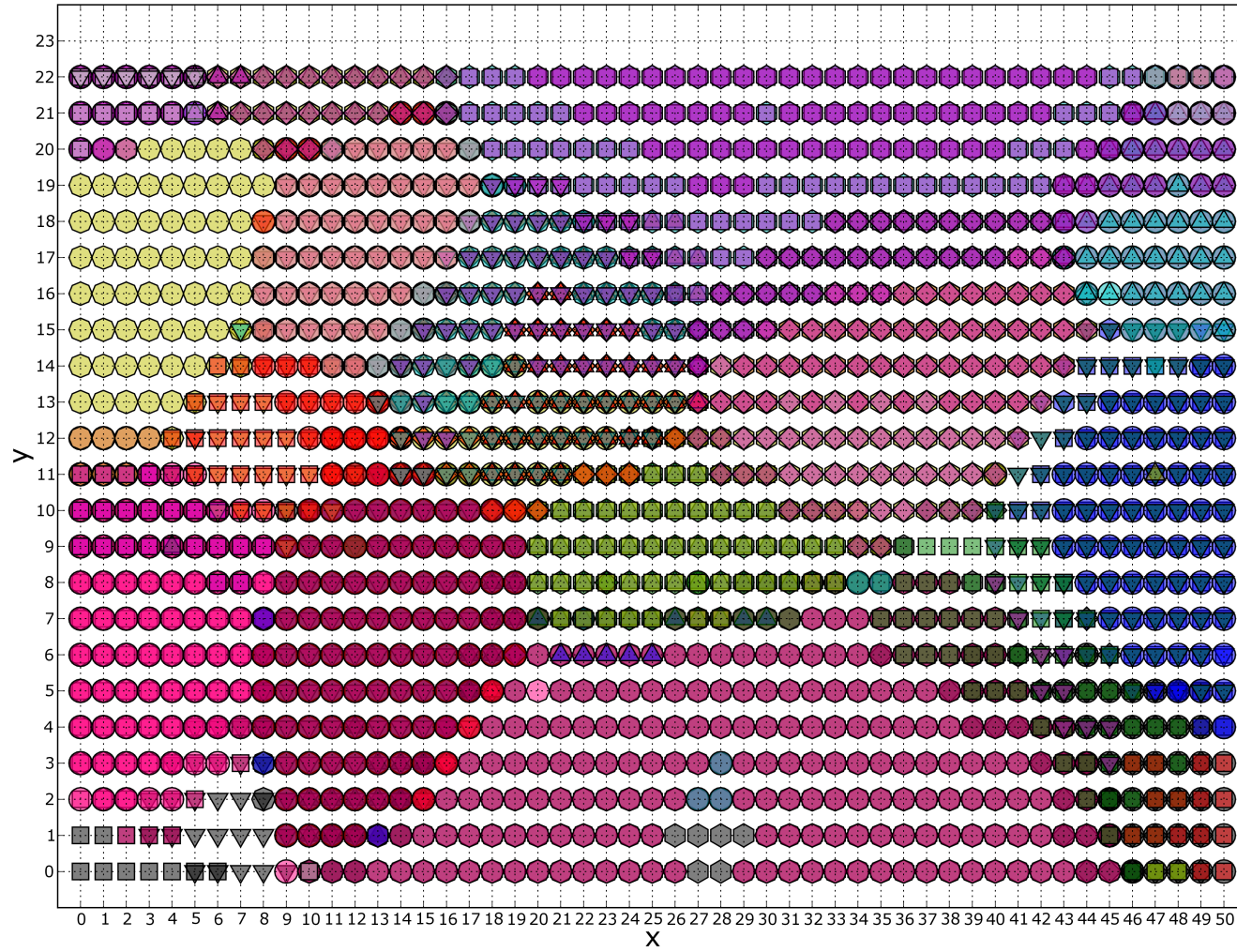
3% tetragonal strain along a^* , b^* , c^*

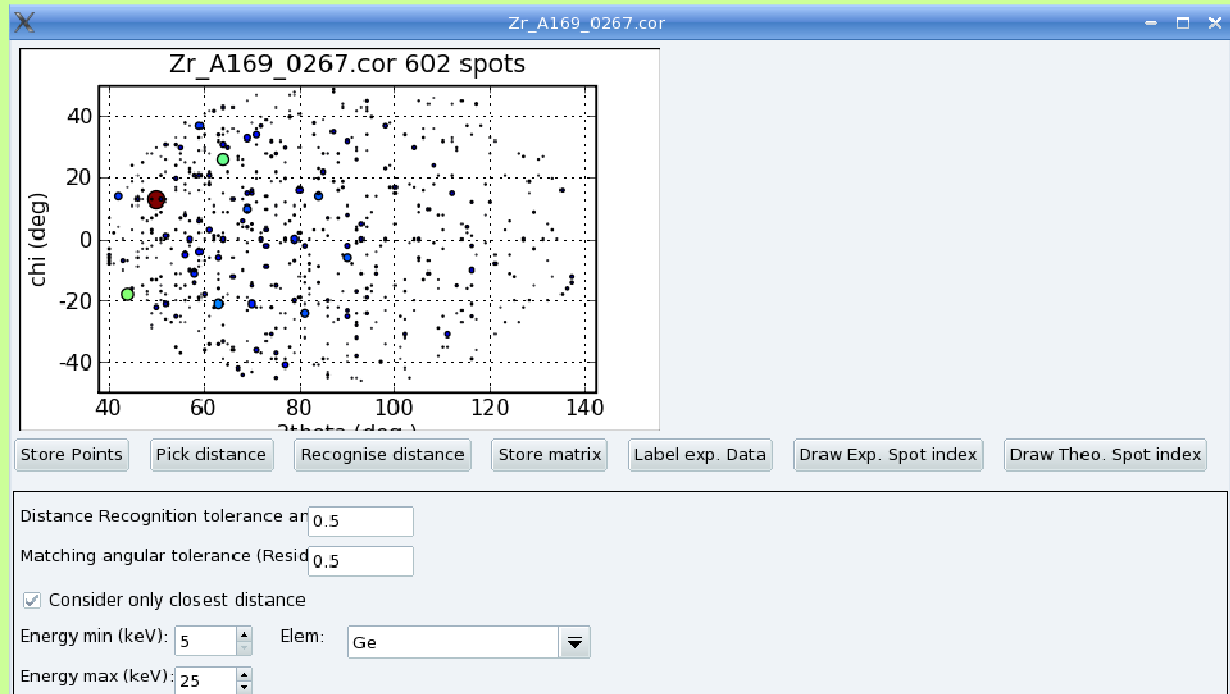


LaueTools Simulation & Indexation Program v1.0 2009									
Zr_A169_0267.cor									
File Plot Calib. Tools Indexation Sequence Simulation Parameters About									
Simulation Data from LAUE Pattern Program v1.0 2009									
spot#	h	k	l	E	2theta	chi	X	Y	
#G	0	Grain_0	0	956					
0	-28	-10	-8	58.30012	130.8445	-128.6598	2730.1702	944.0748	
1	-9	-11	-9	54.14559	64.6871	-129.2894	2745.6740	-521.1022	
2	-11	-7	-1	26.76841	114.5322	-98.1301	2169.8151	393.1338	
3	-17	-9	-9	45.68217	106.3555	-135.0000	2900.7127	353.9036	
4	-3	-7	3	38.45676	43.0009	-66.8014	1682.5517	-994.8315	
5	-24	-10	8	53.09329	123.8318	-51.3402	1365.8298	731.9118	
6	-25	-9	-5	50.34966	135.2338	-119.0546	2521.7293	983.4620	
7	-23	-9	-1	45.74383	137.0197	-96.3402	2142.7459	920.6826	
8	-28	-10	8	58.30012	130.8445	-51.3402	1365.8298	944.0748	
9	-25	-9	5	50.34966	135.2338	-60.9454	1574.2707	983.4620	
10	-10	-10	8	45.45933	75.9703	-51.3402	1365.8298	-272.8681	
11	-7	-5	-5	24.35321	89.4212	-135.0000	2900.7127	-12.1816	
12	-17	-11	5	44.06152	109.1921	-65.5560	1660.4033	326.0372	
13	-11	-7	-7	34.28235	96.0235	-135.0000	2900.7127	127.3532	
14	-9	-11	1	38.83941	78.3478	-84.8056	1970.4807	-176.5718	
15	-17	-13	5	48.92348	101.3433	-68.9625	1720.0336	183.2754	
16	-9	-13	1	48.02312	69.2322	-85.6013	1982.4057	-324.3224	
17	-24	-14	0	55.38921	119.4871	-90.0000	2048.0000	482.1887	
18	-11	-15	3	55.57184	71.4393	-78.6901	1877.4575	-291.9895	
19	-19	-7	3	37.97341	136.3152	-66.8014	1682.5517	971.3231	
20	-13	-9	5	36.42575	103.2436	-60.9454	1574.2707	229.5765	
21	-22	-10	-12	56.98071	109.2488	-140.1944	3071.2553	465.1160	
22	-19	-13	11	58.99925	96.2613	-49.7636	1326.4738	122.5559	
23	-19	-13	-3	48.84885	109.8475	-102.9946	2244.7799	315.8835	
24	-18	-12	4	46.30117	109.8064	-71.5651	1763.7624	323.7150	
25	-12	-6	-2	26.40315	124.4174	-108.4349	2332.2376	615.8481	
26	-11	-11	-1	38.03932	89.7642	-95.1944	2125.5193	-3.5236	
27	-21	-13	5	52.06832	112.8908	-68.9625	1720.0336	385.7510	
28	-15	-15	1	51.77313	89.8730	-86.1859	1991.1525	-1.8949	
29	-13	-15	5	55.49959	78.8536	-71.5651	1763.7624	-177.1019	
30	-18	-12	10	54.33691	98.0957	-50.1944	1337.4051	157.9098	
31	-15	-9	-1	35.24246	117.7519	-96.3402	2142.7459	451.6219	
32	-8	-14	0	55.96319	59.4898	-90.0000	2048.0000	-502.4914	
33	-14	-12	-12	59.53008	79.0424	-135.0000	2900.7127	-233.4809	
34	-5	-9	-5	45.11494	51.8054	-119.0546	2521.7293	-767.4415	
35	-10	-4	-2	20.66333	131.8103	-116.5651	2474.3564	852.7127	
36	-4	-4	2	15.49750	83.6206	-63.4349	1621.6436	-106.5891	
37	-19	-7	-5	39.42346	131.2823	-125.5377	2657.0805	920.0322	
38	-15	-11	5	42.58943	102.2246	-65.5560	1660.4033	204.1343	



UO2_He: Major spots presence map





Classical Indexation Board :Zr_A169_0267.cor

Parameters Current File: Zr_A169_0267.cor

Energy max.: 25

Element: UO2

Intense spots set Size (ISSS): 10

List of spots index: [0,5,6]
(from 0 to ISSS-1)

Dist. Recogn. Tol. Angle (deg): 0.5

Matching Tolerance Angle (deg): 0.2

Minimum Number Matched Spots: 15

Plot Best results Number best results plotted: 3

Start Quit

Human-aided indexing

Potential solutions

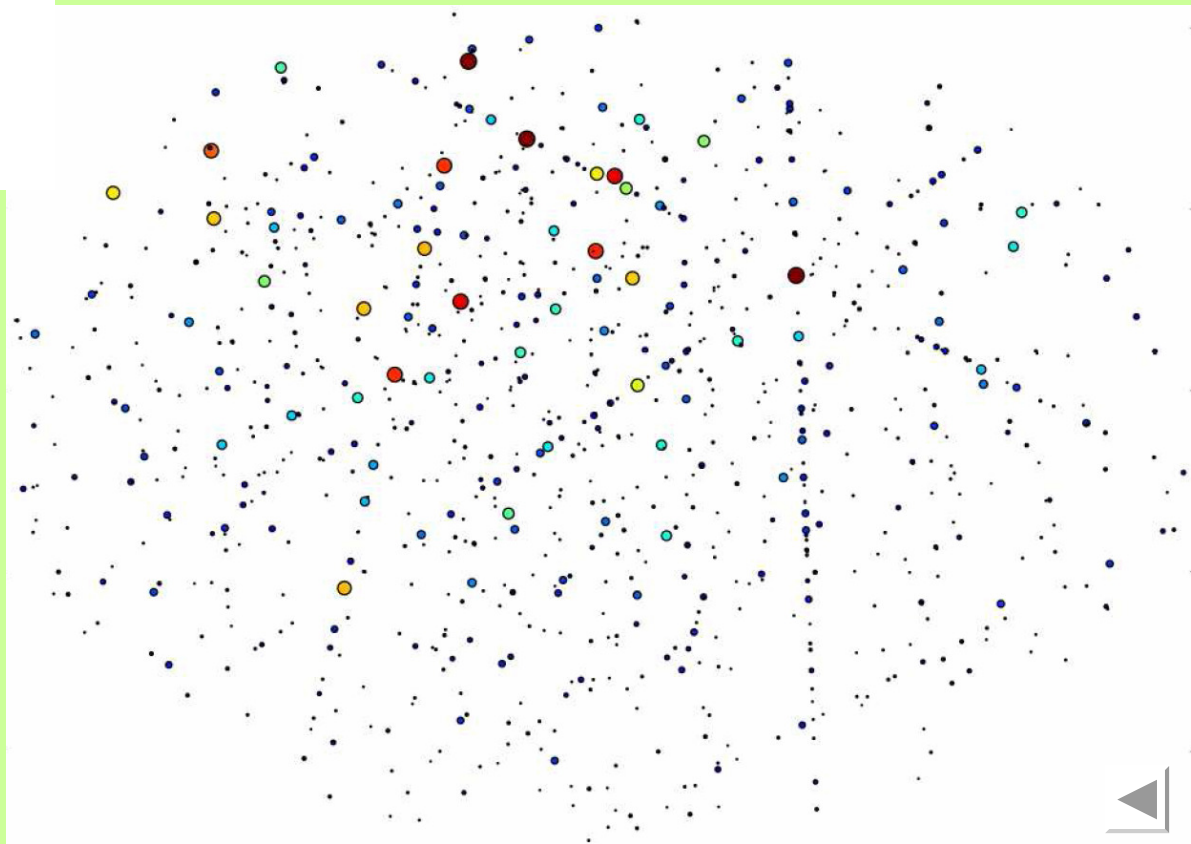
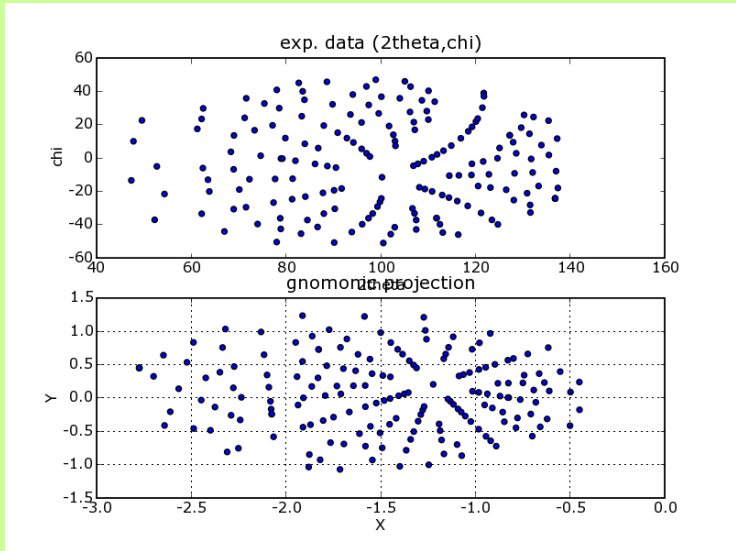
	#Matrix	nb. <MTAR=0.50	nb. <DRTA=0.50	mean	max
<input checked="" type="checkbox"/>	0	36	248	0.327	0.496
<input type="checkbox"/>	1	27	245	0.305	0.493
<input type="checkbox"/>	2	33	258	0.313	0.485
<input type="checkbox"/>	3	42	257	0.324	0.498

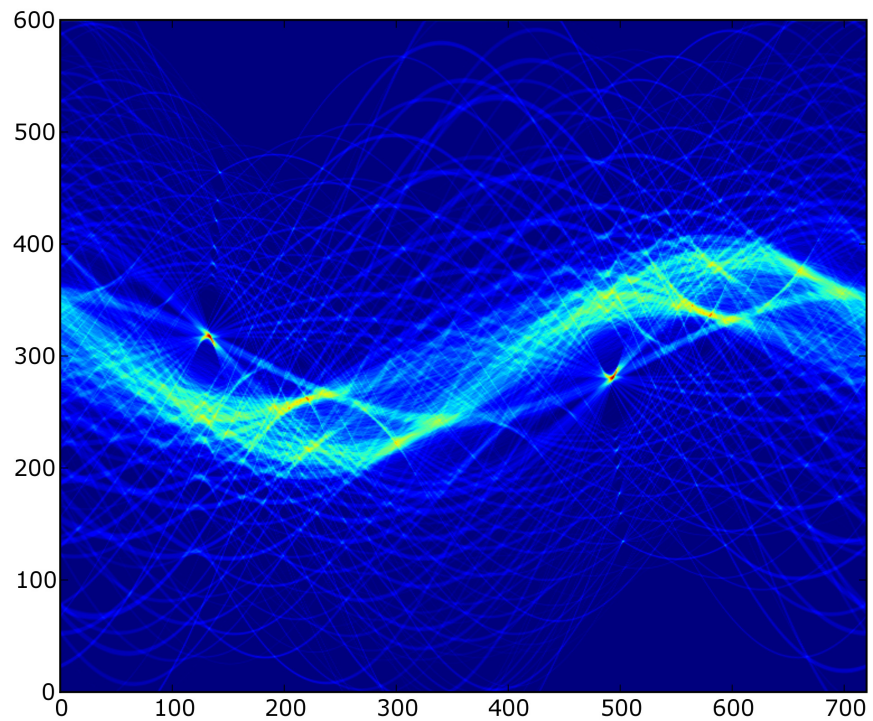
Energy min: 5 Energy max: 25

Plot Simul S3 Quit

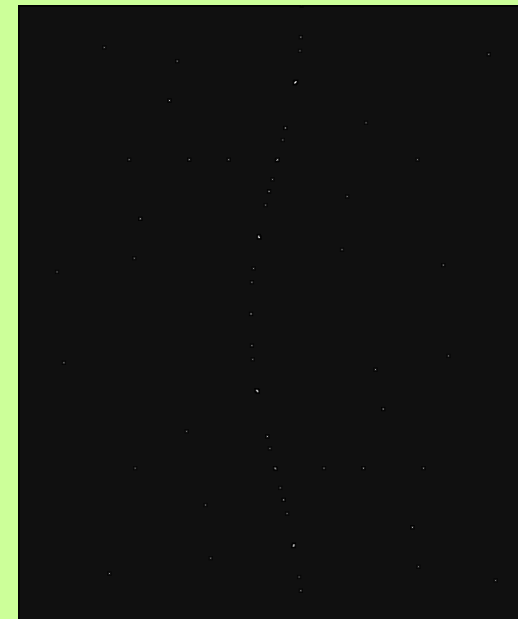
Automatic indexing







Data 27000 most intense pixel

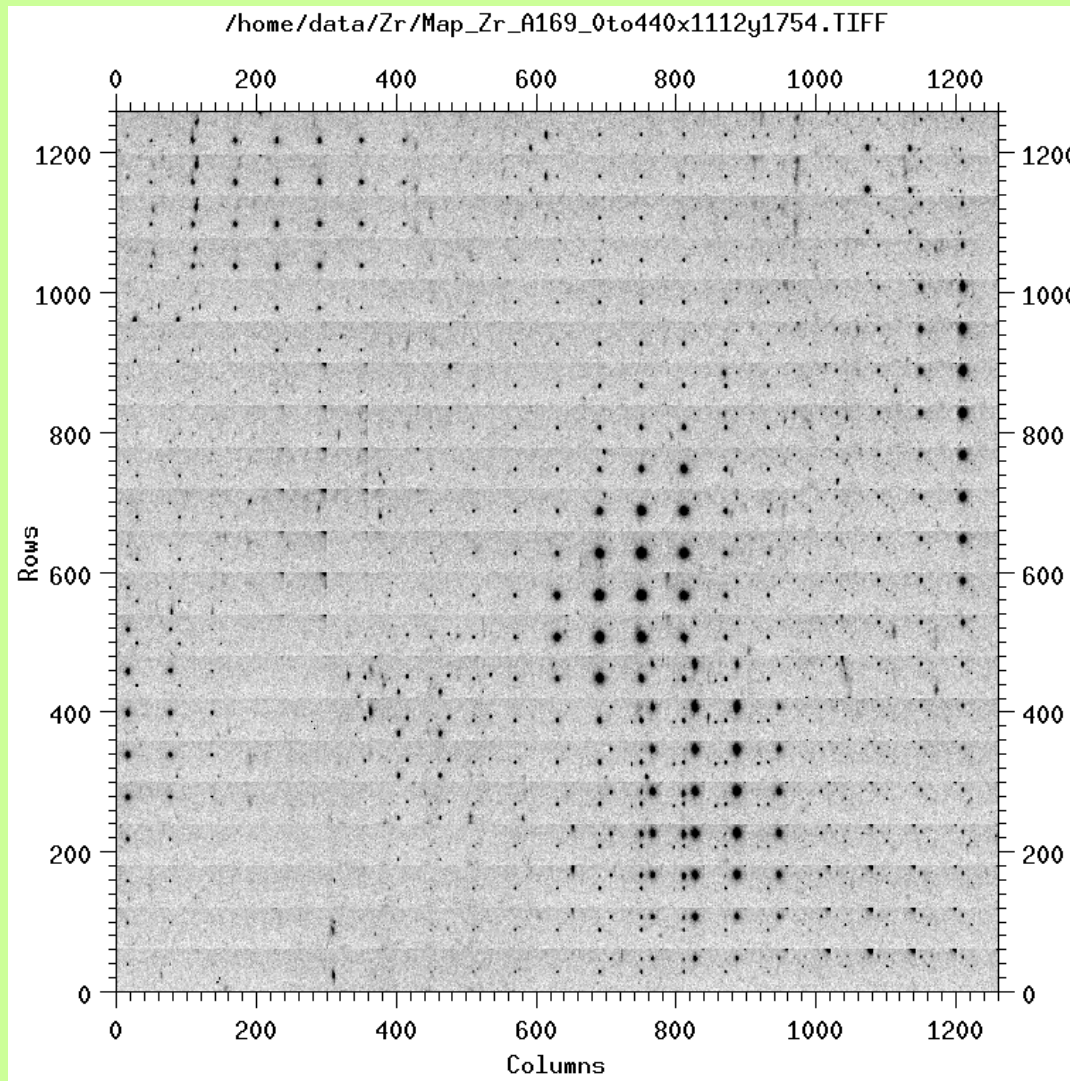


Fingerprint of one crystal orientation:
 ϕ_1, ϕ_2, ϕ_3

Only few non zeros pixels



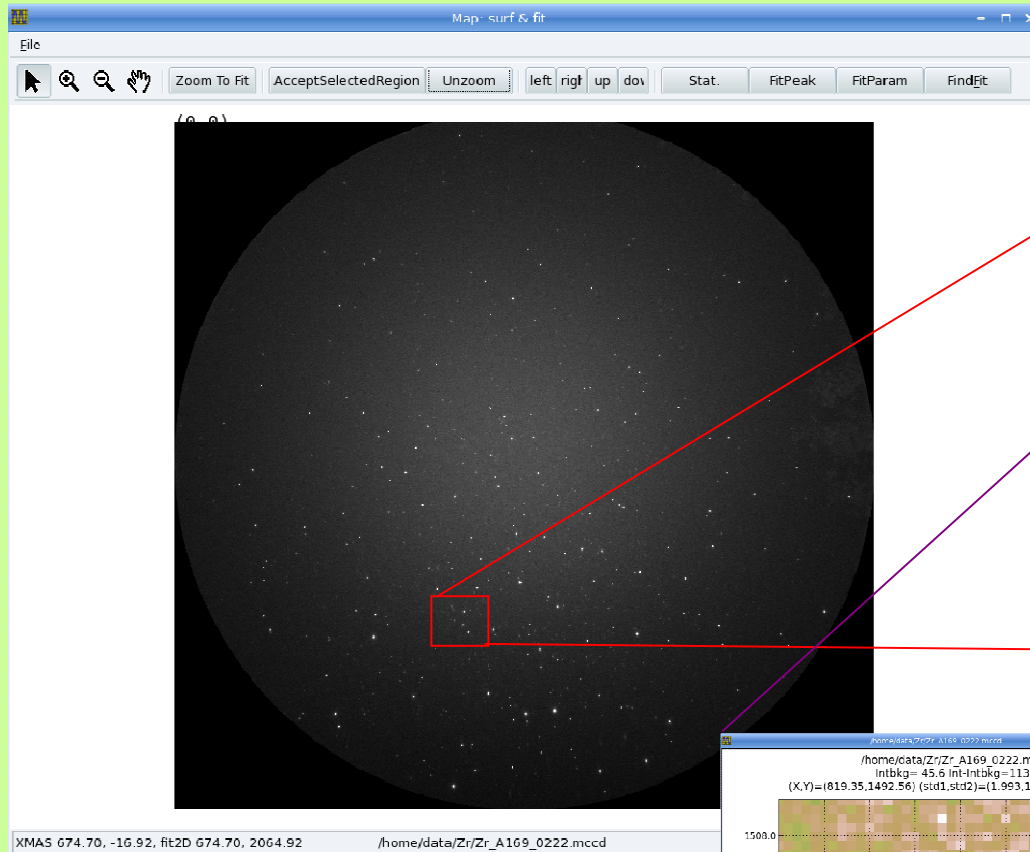
mosaic



2D microLaue pattern ROI
Grain mapping



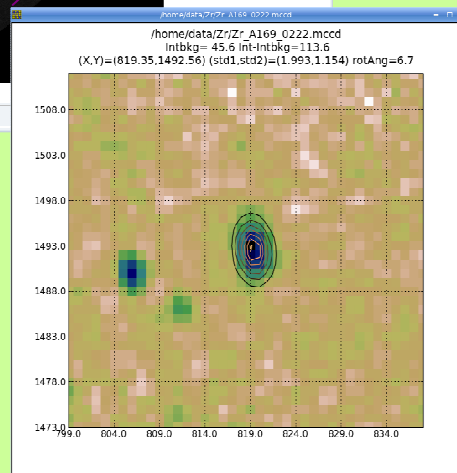
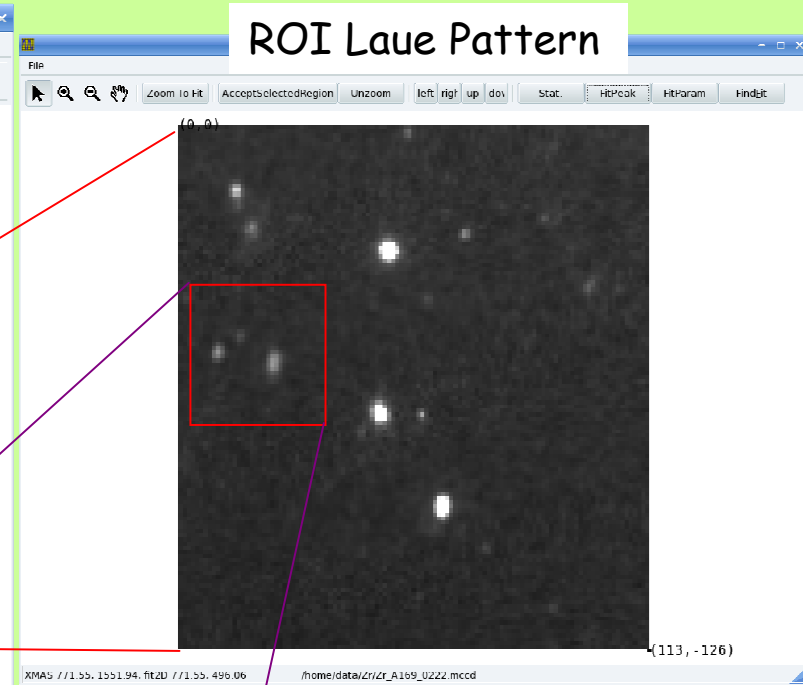
Images set navigator & processing



Navigation on images dataset : Full Pattern

Mapcanvas.py

fit2Dintensity.py



2D intensity fitting

results, batchable

