

NAME

pyFAI-recalib – pyFAI-recalib

DESCRIPTION

INFO:root:Enter, port=54321. INFO:root:Enter. usage: pyFAI-recalib [options] **-p** ponifile **-w** 1 **-c** calibrant.D imagefile.edf

Calibrate the diffraction setup geometry based on Debye–Sherrer rings images with a priori knowledge of your setup (an input PONI–file). You will need to provide a calibrant or a "d–spacing" file containing the spacing of Miller plans in Angstrom (in decreasing order). Calibrants available: quartz, Cr2O3, AgBh, CrOx, C14H30O, ZnO, Al, NaCl, cristobaltite, Si, Au, LaB6, CeO2, PBBA, alpha_Al2O3 or search in the American Mineralogist database: <http://rruff.geo.arizona.edu/AMS/amcsd.php> The **–calibrant** option is mandatory !

positional arguments:

FILE List of files to calibrate

optional arguments:

-h, --help

show this help message and exit

-V, --version

show program's version number and exit

-o FILE, --out FILE

Filename where processed image is saved

-v, --verbose

switch to debug/verbose mode

-c FILE, --calibrant FILE

Calibrant name or file containing d–spacing of the reference sample (MANDATORY, case sensitive !)

-w WAVELENGTH, --wavelength WAVELENGTH

wavelength of the X–Ray beam in Angstrom. Mandatory

-e ENERGY, --energy ENERGY

energy of the X–Ray beam in keV ($hc=12.398419292keV.A$).

-P POLARIZATION_FACTOR, --polarization POLARIZATION_FACTOR

polarization factor, from **-1** (vertical) to **+1** (horizontal), default is None (no correction), synchrotrons are around 0.95

-b BACKGROUND, --background BACKGROUND

Automatic background subtraction if no value are provided

-d DARK, --dark DARK

list of comma separated dark images to average and subtract

-f FLAT, --flat FLAT

list of comma separated flat images to average and divide

-s SPLINE, --spline SPLINE

spline file describing the detector distortion

-D DETECTOR_NAME, --detector DETECTOR_NAME

Detector name (instead of pixel size+spline)

-m MASK, --mask MASK

file containing the mask (for image reconstruction)

-n NPT, --pt NPT

file with datapoints saved. Default: basename.npt

- filter** FILTER
select the filter, either mean(default), max or median
- l** DISTANCE, **--distance** DISTANCE
sample-detector distance in millimeter. Default: 100mm
- dist** DIST
sample-detector distance in meter. Default: 0.1m
- poni1** PONI1
poni1 coordinate in meter. Default: center of detector
- poni2** PONI2
poni2 coordinate in meter. Default: center of detector
- rot1** ROT1
rot1 in radians. default: 0
- rot2** ROT2
rot2 in radians. default: 0
- rot3** ROT3
rot3 in radians. default: 0
- fix-dist**
fix the distance parameter
- free-dist**
free the distance parameter. Default: Activated
- fix-poni1**
fix the poni1 parameter
- free-poni1**
free the poni1 parameter. Default: Activated
- fix-poni2**
fix the poni2 parameter
- free-poni2**
free the poni2 parameter. Default: Activated
- fix-rot1**
fix the rot1 parameter
- free-rot1**
free the rot1 parameter. Default: Activated
- fix-rot2**
fix the rot2 parameter
- free-rot2**
free the rot2 parameter. Default: Activated
- fix-rot3**
fix the rot3 parameter
- free-rot3**
free the rot3 parameter. Default: Activated
- fix-wavelength**
fix the wavelength parameter. Default: Activated
- free-wavelength**
free the wavelength parameter. Default: Deactivated
- tilt** Allow initially detector tilt to be refined (rot1, rot2, rot3). Default: Activated

- no-tilt**
Deactivated tilt refinement and set all rotation to 0
- saturation SATURATION**
consider all pixel>max*(1-saturation) as saturated and reconstruct them, default: 0 (deactivated)
- weighted**
weight fit by intensity, by default not.
- npt NPT_1D**
Number of point in 1D integrated pattern, Default: 1024
- npt-azim NPT_2D_AZIM**
Number of azimuthal sectors in 2D integrated images. Default: 360
- npt-rad NPT_2D_RAD**
Number of radial bins in 2D integrated images. Default: 400
- unit UNIT**
Valid units for radial range: 2th_deg, 2th_rad, q_nm⁻¹, q_A⁻¹, r_mm. Default: 2th_deg
- no-gui**
force the program to run without a Graphical interface
- no-interactive**
force the program to run and exit without prompting for refinements
- r MAX_RINGS, --ring MAX_RINGS**
maximum number of rings to extract. Default: all accessible
- p FILE, --poni FILE**
file containing the diffraction parameter (poni-file). MANDATORY
- k, --keep**
Keep existing control point and append new

The main difference with pyFAI-calib is the way control-point hence DebyeSherrer rings are extracted. While pyFAI-calib relies on the contiguity of a region of peaks called massif; pyFAI-recalib knows approximately the geometry and is able to select the region where the ring should be. From this region it selects automatically the various peaks; making pyFAI-recalib able to run without graphical interface and without human intervention (**--no-gui** and **--nointeractive** options). Note that 'pyFAI-recalib' program is obsolete as the same fonctionnality is available from within pyFAI-calib, using the 'recalib' command in the refinement process. Two option are available for recalib: the numbe of rings to extract (similar to the **-r** option of this program) and a new option which lets you choose between the original 'massif' algorithm and newer ones like 'blob' and 'watershed' detection.