NAME

pyFAI-calib − Calibration tool

DESCRIPTION

usage: pyFAI−calib [options] **−w** 1 **−D** detector **−c** calibrant.D imagefile.edf

Calibrate the diffraction setup geometry based on Debye−Sherrer rings images without a priori knowledge of your setup. 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: Ni, CrOx, NaCl, Si_SRM640e, Si_SRM640d, Si_SRM640a, Si_SRM640c, alpha_Al2O3, Cr2O3, TiO2, Si_SRM640, CuO, PBBA, Si_SRM640b, mock, quartz, C14H30O, cristobaltite, Si, LaB6, CeO2, LaB6_SRM660a, LaB6_SRM660b, LaB6_SRM660c, AgBh, ZnO, Al, Au 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

−i FILE, **−−poni** FILE
file containing the diffraction parameter (poni−file). MANDATORY for pyFAI−recalib!

−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_nmˆ−1, q_Aˆ−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, **−−reconstruct**
Reconstruct image where data are masked or <0 (for Pilatus detectors or detectors with modules)

−g GAUSSIAN, **−−gaussian** GAUSSIAN
Size of the gaussian kernel. Size of the gap (in pixels) between two consecutive rings, by default 100 Increase the value if the arc is not complete; decrease the value if arcs are mixed together.

−−square
Use square kernel shape for neighbor search instead of diamond shape

−p PIXEL, **−−pixel** PIXEL
size of the pixel in micron

The output of this program is a "PONI" file containing the detector description and the 6 refined parameters (distance, center, rotation) and wavelength. An 1D and 2D diffraction patterns are also produced. (.dat and .azim files)