NAME

pyFAI-calib − pyFAI-calib

SYNOPSIS

pyFAI-calib [*options*] *-w 1 -D detector -S calibrant.D imagefile.edf*

DESCRIPTION

Calibrate the diffraction setup geometry based on Debye−Sherrer rings images without a priori knowledge of your setup. You will need a "d−spacing" file containing the spacing of Miller plans in Angstrom (in decreasing order). If you are using a standart calibrant, look at https://github.com/kif/pyFAI/tree/master/calibration or search in the American Mineralogist database: http://rruff.geo.arizona.edu/AMS/amcsd.php

OPTIONS

−−version
show program's version number and exit

−h, **−−help**
show this help message and exit

−o FILE, **−−out**=*FILE*
Filename where processed image is saved

−v, **−−verbose**
switch to debug/verbose mode

−S FILE, **−−spacing**=*FILE*
file containing d−spacing of the reference sample (MANDATORY)

−w WAVELENGTH, **−−wavelength**=*WAVELENGTH*
wavelength of the X−Ray beam in Angstrom

−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 dark images to average and subtract

−f FLAT, **−−flat**=*FLAT*
list of 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

−−poni1=*PONI1*
poni1 coordinate in meter

−−poni2=*PONI2*
poni2 coordinate in meter

−−rot1=*ROT1*
rot1 in radians

−−rot2=*ROT2*
rot2 in radians

−−rot3=*ROT3*
rot3 in radians

−−fix−dist
fix the distance parameter

−−free−dist
free the distance parameter

−−fix−poni1
fix the poni1 parameter

−−free−poni1
free the poni1 parameter

−−fix−poni2
fix the poni2 parameter

−−free−poni2
free the poni2 parameter

−−fix−rot1
fix the rot1 parameter

−−free−rot1
free the rot1 parameter

−−fix−rot2
fix the rot2 parameter

−−free−rot2
free the rot2 parameter

−−fix−rot3
fix the rot3 parameter

−−free−rot3
free the rot3 parameter

−−fix−wavelength
fix the wavelength parameter

−−free−wavelength
free the wavelength parameter

−−saturation=*SATURATION*
consider all pixel>max*(1−saturation) as saturated and reconstruct them

−−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.

−c, **−−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)