### **NAME**

pyFAI-recalib – pyFAI-recalib

## **DESCRIPTION**

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 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

# positional arguments:

FILE List of files to calibrate

### optional arguments:

## -h, --help

show this help message and exit

### -V, --version

### -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)

## -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

 $free\ the\ rot 3\ parameter$ 

# --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\_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 approximatly 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).

PyFAI June 2014 3