#### **NAME**

pyFAI-recalib - Deprecated

## **DESCRIPTION**

usage: pyFAI-recalib [options] -i 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: Ni, CrOx, NaCl, Si\_SRM640e, Si\_SRM640d, Si\_SRM640e, alpha\_Al2O3, Cr2O3, TiO2, Si\_SRM640, CuO, PBBA, Si\_SRM640b, quartz, C14H30O, cristobaltite, Si, LaB6, CeO2, moke, 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\_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

### -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). Note that 'pyFAI–recalib' program is obsolete as the same functionality 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.