
xrayutilities Documentation

Release 0.99.1

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July 03, 2013

CONTENTS

1	Introduction	3
1.1	Concept of usage	4
1.2	Angle calculation using the material classes	5
1.3	hello world	5
2	xrayutilities Python package	9
3	Installation	11
3.1	Express instructions	11
3.2	Detailed instructions	11
3.3	Required third party software	11
3.4	Building and installing the library and python package	12
3.5	Setup of the Python package	12
3.6	Notes for installing on Windows	12
4	Examples and API-documentation	15
4.1	Examples	15
4.2	xrayutilities Package	24
4.3	analysis Package	74
4.4	io Package	87
4.5	materials Package	96
4.6	math Package	105
4.7	xrayutilities	110
5	Indices and tables	161
	Python Module Index	163
	Index	165

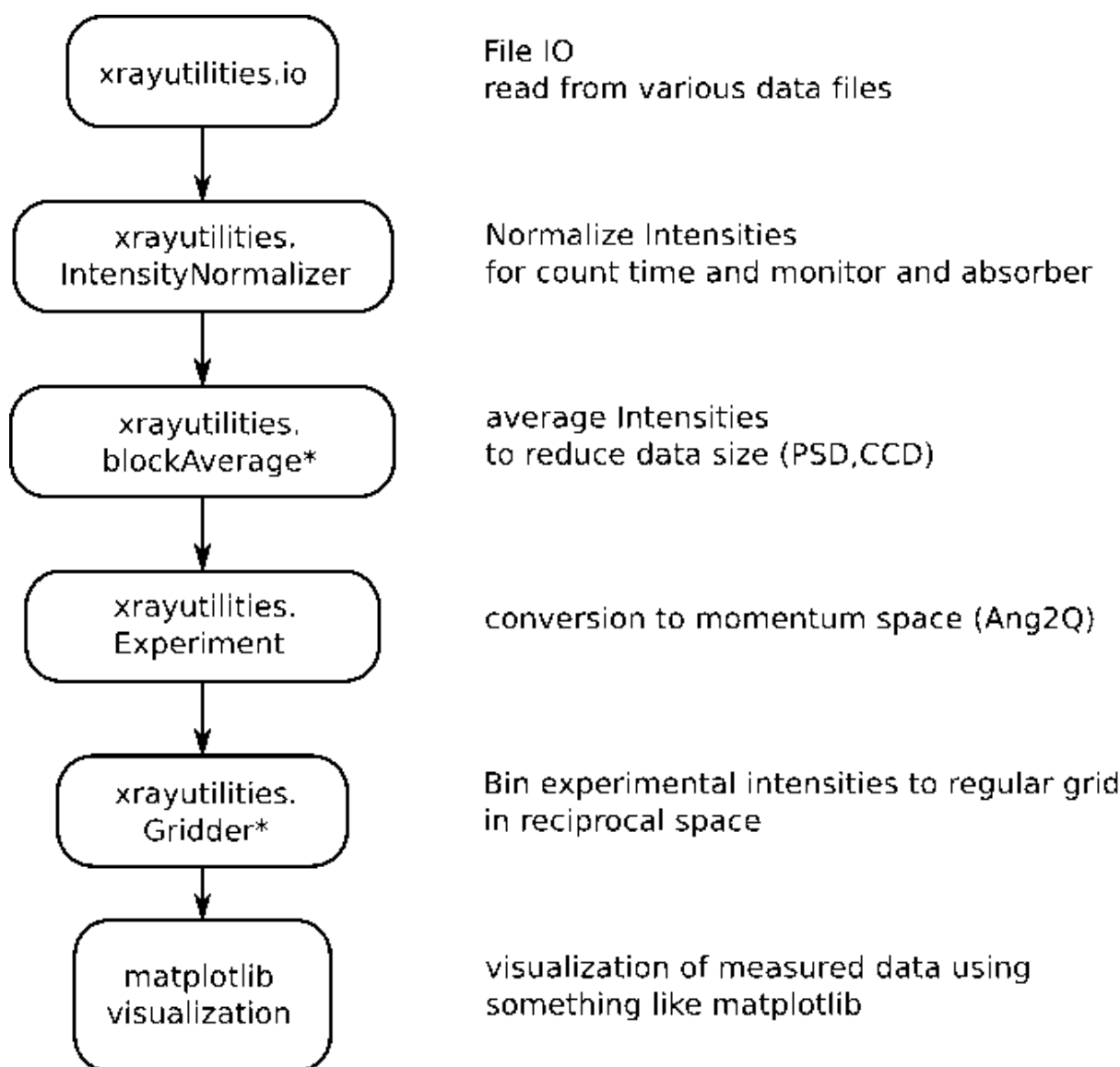
If you look for downloading the package go [here](#). Installation instructions you find further down [Installation](#).

INTRODUCTION

xrayutilities is a collection of scripts used to analyze x-ray diffraction data. It consists of a python package and several routines coded in C. It is especially useful for the reciprocal space conversion of diffraction data taken with linear and area detectors.

In the following two concepts of usage for the *xrayutilities* package will be described. First one should get a brief idea of how to analyze x-ray diffraction data with *xrayutilities*. After that the concept of how angular coordinates of Bragg reflections are calculated is presented.

1.1 Concept of usage



xrayutilities provides a set of functions to read experimental data from various data file formats. All of them are gathered in the `io`-subpackage. After reading data with a function from the `io`-submodule the data might be corrected for monitor counts and/or absorption factor of a beam attenuator. A special set of functions is provided to perform this for point, linear and area detectors.

Since the amount of data taken with modern detectors often is too large to be able to work with them properly, a functions for reducing the data from linear and area detectors are provided. They use block-averaging to reduce the amount of data. Use those carefully not to loose the features you are interested in in your measurements.

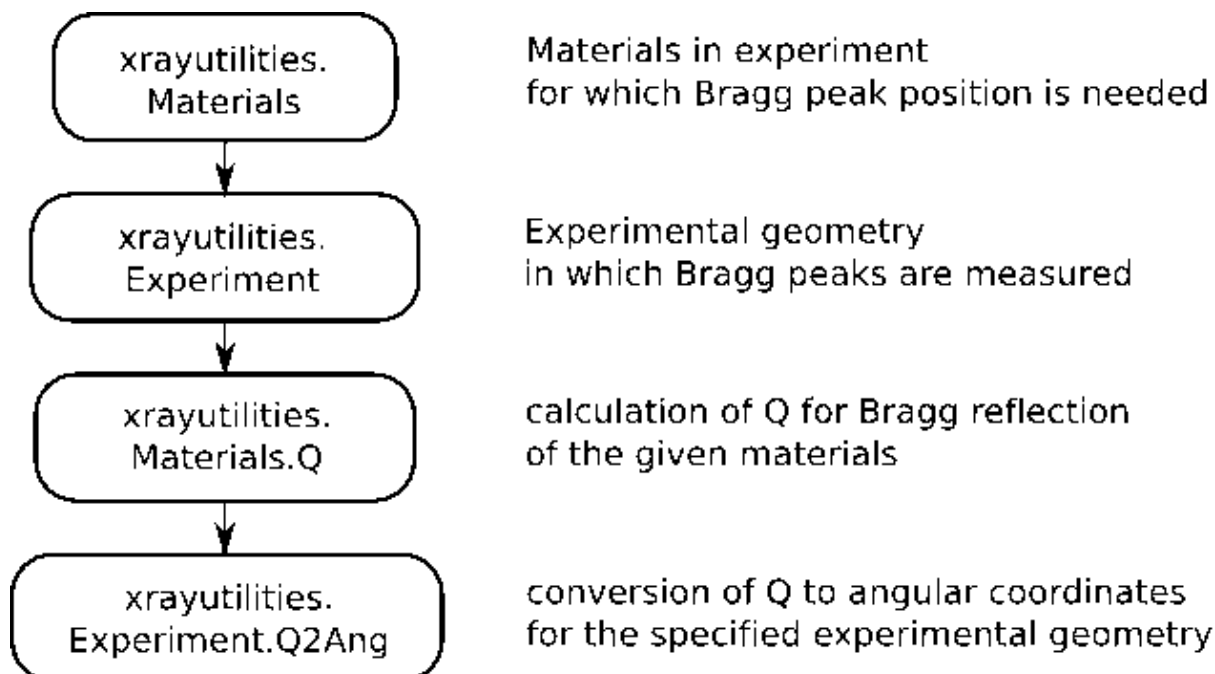
After the pre-treatment of the data, the core part of the package is the transformation of the angular data to reciprocal space. This is done as described in more detail below using the `experiment-module`. The classes provided within the `experiment` module provide routines to help performing X-ray diffraction experiments. This includes methods to calculate the diffraction angles (described below) needed to align crystalline samples and to convert data between angular and reciprocal space. The conversion from angular to reciprocal space is implemented very general for various goniometer geometries. It is especially useful in combination with linear and area detectors as described in this [article](#). In standard cases, Users will only need the initialized routines, which predefine a certain goniometer geometry like the popular four-circle and six-circle geometries.

After the conversion to reciprocal space, it is convenient to transform the data to a regular grid for visualization. For this purpose the `gridder`-module has been included into *xrayutilities*. For the visualization of the data in

reciprocal space the usage of `matplotlib` is recommended.

A practical example showing the usage is given below.

1.2 Angle calculation using the material classes



Calculation of angles needed to align Bragg reflections in various diffraction geometries is done using the Materials defined in the `materials`-package. This package provides a set of classes to describe crystal lattices and materials. Once such a material is properly defined one can calculate its properties, which includes the reciprocal lattice points, optical properties like the refractive index, the structure factor (including the atomic scattering factor) and the complex polarizability. These atomic properties are extracted from a database included in `xrayutilities`.

Using such a material and an experimental class from the `experiment`-module describing the experimental setup the needed diffraction angles can be calculated for certain coplanar diffraction (high, low incidence), grazing incidence diffraction and also special non-coplanar diffraction geometries.

1.3 hello world

A first example with step by step explanation is shown in the following. It showcases the use of `xrayutilities` to calculate angles and read a scan recorded with a linear detector from `spec`-file and plots the result as reciprocal space map using `matplotlib`.

```

1  """
2  Example script to show how to use xrayutilities to read and plot
3  reciprocal space map scans from a spec file created at the ESRF/ID10B
4
5  for details about the measurement see:
6      D Kriegner et al. Nanotechnology 22 425704 (2011)
7      http://dx.doi.org/10.1088/0957-4484/22/42/425704
8  """
9
10 import numpy
11 import matplotlib.pyplot as plt
12 import xrayutilities as xu
13 import os

```

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```
# global setting for the experiment
sample = "test" # sample name used also as file name for the data file
energy = 8042.5 # x-ray energy in eV
center_ch = 715.9 # center channel of the linear detector
chpdeg = 345.28 # channels per degree of the linear detector
roi=[100,1340] # region of interest of the detector
nchannel = 1500 # number of channels of the detector

# intensity normalizer function responsible for count time and absorber correction
absfun = lambda d: d["detcorr"]/d["psd2"].astype(numpy.float)
normalizer_detcorr = xu.IntensityNormalizer("MCA",mon="Monitor",time="Seconds",absfun=absfun)

# substrate material used for Bragg peak calculation to correct for experimental offsets
InP = xu.materials.InP

# initialize experimental class to specify the reference directions of your crystal
# 11-2: inplane reference
# 111: surface normal
hxr = xu.HXRD(InP.Q(1,1,-2),InP.Q(1,1,1),en=energy)

# configure linear detector
# detector direction + parameters need to be given
# mounted along z direction, which corresponds to twotheta
hxr.Ang2Q.init_linear('z-',center_ch,nchannel,chpdeg=chpdeg,roi=roi)

# read spec file and save to HDF5-file
# since reading is much faster from HDF5 once the data are transformed
h5file = os.path.join("data",sample+".h5")
try: s = xu.io.SPECFile(sample+".spec",path="data")
except NameError: s = xu.io.SPECFile(sample+".spec",path="data")
else: s.Update()
s.Save2HDF5(h5file)

#####
# InP (333) reciprocal space map
omalign = 43.0529 # experimental aligned values
ttalign = 86.0733
[omnominal,dummy,dummy,ttnominal] = hxr.Q2Ang(InP.Q(3,3,3)) # nominal values of the substrate pe

# read the data from the HDF5 file
#(scan number:36, names of motors in spec file: omega= sample rocking, gamma = twotheta)
[om,tt],MAP = xu.io.get_h5_scan(h5file,36,'omega','gamma')
# normalize the intensity values (absorber and count time corrections)
psdraw = normalizer_detcorr(MAP)
# remove unusable detector channels/regions (no averaging of detector channels)
psd = xu.blockAveragePSD(psdraw, 1, roi=roi)

# convert angular coordinates to reciprocal space + correct for offsets
[qx,qy,qz] = hxr.Ang2Q.linear(om,tt,delta=[omalign-omnominal, ttalign-ttnominal])

# calculate data on a regular grid of 200x201 points
gridder = xu.Gridder2D(200,201)
gridder(qx,qz,psd)
# maplog function limits the shown dynamic range to 8 orders of magnitude from the maxium
INT = xu.maplog(gridder.gdata.transpose(),8.,0)

# plot the intensity as contour plot using matplotlib
plt.figure()
cf = plt.contourf(gridder.xaxis, gridder.yaxis,INT,100,extend='min')
plt.xlabel(r'$Q_{[11\bar{2}]}$ ($\AA^{-1}$)')
plt.ylabel(r'$Q_{[\bar{1}1\bar{1}]}$ ($\AA^{-1}$)')
cb = plt.colorbar(cf)
```

```
77 cb.set_label(r"$\log($Int$)$ (cps)")
```

More such examples can be found on the *Examples* page.

XRAYUTILITIES PYTHON PACKAGE

xrayutilities is a Python package for assisting with x-ray diffraction experiments. Its the python package included in *xrayutilities*.

It helps with planning experiments as well as analyzing the data.

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for more details see the full API documentation of `xrayutilities` found here: *[Examples and API-documentation](#)*.

INSTALLATION

3.1 Express instructions

- install the dependencies (Windows: [pythonxy](#); Linux/Unix: see below for dependencies).
- download *xrayutilities* from [here](#) or use git to check out the [latest](#) version.
- open a command line and navigate to the downloaded sources and execute:

```
> python setup.py install
```

which will install *xrayutilities* to the default directory. It should be possible to use it (*import xrayutilities*) from now on in python scripts.

Note: The python package of *xrayutilities* was formerly called ‘xrutils’

3.2 Detailed instructions

Installing *xrayutilities* is done using Python’s distutils

The package can be installed on Linux, Mac OS X and Microsoft Windows, however it is mostly tested on Linux/Unix platforms. Please inform one of the authors in case the installation fails!

3.3 Required third party software

To keep the coding effort as small as possible *xrayutilities* depends on a large number of third party libraries and Python modules.

The needed dependencies are:

- **GCC** Gnu Compiler Collection or any compatible C compiler. On windows you most probably should use MinGW or CygWin. Others might work but are untested.
- **HDF5** a versatile binary data format (library is implemented in C). Although the library is not called directly, it is needed by the pytables Python module (see below).
- **Python** the scripting language in which most of *xrayutilities* code is written in.
- **git** a version control system used to keep track on the *xrayutilities* development. (only needed for development)

Additionally, the following Python modules are needed in order to make *xrayutilities* work as intended:

- **Numpy** a Python module providing numerical array objects
- **Scipy** a Python module providing standard numerical routines, which is heavily using numpy arrays

- **Python-Tables** a powerful Python interface to HDF5.
- **Matplotlib** a Python module for high quality 1D and 2D plotting (optionally)
- **IPython** although not a dependency of *xrayutilities* the IPython shell is perfectly suited for the interactive use of the *xrayutilities* python package.

After installing all required packages you can continue with installing and building the C library.

3.4 Building and installing the library and python package

xrayutilities uses the distutils packaging system to build and install all of its components. You can perform the installation by executing

```
>python setup.py install
```

or

```
>python setup.py install --prefix=INSTALLPATH
```

in the root directory of the source distribution.

The *--prefix* option sets the root directory for the installation. If it is omitted the library is installed under */usr/lib/* on Unix systems or in the Python installation directory on Windows.

3.5 Setup of the Python package

You need to make your Python installation aware of where to look for the module. This is usually only needed when installing in non-standard *<install path>* locations. For this case append the installation directory to your *PYTHONPATH* environment variable by

```
>export PYTHONPATH=$PYTHONPATH:<local install path>/lib64/python2.7/site-packages
```

on a Unix/Linux terminal. Or, to make this configuration persistent append this line to your local *.bashrc* file in your home directory. On MS Windows you would like to create a environment variable in the system preferences under system in the advanced tab (Using pythonxy this is done automatically). Be sure to use the correct directory which might be similar to

```
<local install path>/Lib/site-packages
```

on Windows systems.

3.6 Notes for installing on Windows

Since there is no packages manager on Windows the packages need to be installed manual (including all the dependencies) or a pre-packed solution needs to be used. We strongly suggest to use the *python(x,y)* python distribution, which includes already all of the needed dependencies for installing *xrayutilities*.

The setup of the environment variables is also done by the *python(x,y)* installation. One can proceed with the installation of *xrayutilities* directly!

In case you want to do it the hard way install all of the following (versions in brackets indicate the tested set of versions by the

- MinGW (0.4alpha)
- Python (2.7.2)
- numpy (1.6.1)

- scipy (0.10.1)
- numexpr (1.4.2) needed for pytables
- pytables (2.3.1)
- matplotlib (1.1.0)
- ipython (0.12)

It is suggested to add the MinGW binary directory, as well as the Python and Python-scripts directory to the Path environment variable as described above! Installation is done as described above.

EXAMPLES AND API-DOCUMENTATION

4.1 Examples

In the following a few code-snippets are shown which should help you getting started with *xrayutilities*. Not all of the codes shown in the following will be run-able as stand-alone script. For fully running scripts look in the `examples` directory in the download found [here](#).

4.1.1 Reading data from data files

The `io` submodule provides classes for reading x-ray diffraction data in various formats. In the following few examples are given.

Reading SPEC files

Working with spec files in *xrayutilities* can be done in two distinct ways.

1. parsing the spec file for scan headers; and parsing the data only when needed
2. parsing the spec file for scan headers; parsing all data and dump them to an HDF5 file; reading the data from the HDF5 file.

Both methods have their pros and cons. For example when you parse the spec-files over a network connection you need to re-read the data again over the network if using method 1) whereas you can dump them to a local file with method 2). But you will parse data of the complete file while dumping it to the HDF5 file.

Both methods work incremental, so they do not start at the beginning of the file when you reread it, but start from the last position they were reading and work with files including data from linear detectors.

An working example for both methods is given in the following.:

```
1 import tables
2 import xrayutilities as xu
3 import os
4
5 # open spec file or use open SPECfile instance
6 try: s
7 except NameError:
8     s = xu.io.SPECFile("sample_name.spec", path="./specdir")
9
10 # method (1)
11 scan10 = s[9] # Returns a SPECScan class, note 9 because the list starts at 0
12 scan10.ReadData()
13 scan10data = scan10.data
14
```

```
15 # method (2)
16 h5file = os.path.join("h5dir","h5file.h5")
17 s.Save2HDF5(h5file) # save content of SPEC file to HDF5 file
18 # read data from HDF5 file
19 [angle1,angle2],scan10data = xu.io.geth5_scan(h5file,[10], "motorname1", "motorname2")
```

See Also:

the fully working example *hello world*

In the following it is shown how to re-parsing the SPEC file for new scans and reread the scans (1) or update the HDF5 file(2)

```
1 s.Update() # reparse for new scans in open SPECFile instance
2
3 # reread data method (1)
4 scan10 = s[9] # Returns a SPECScan class
5 scan10.ReadData()
6 scan10data = scan10.data
7
8 # reread data method (2)
9 s.Save2HDF5(h5) # save content of SPEC file to HDF5 file
10 # read data from HDF5 file
11 [angle1,angle2],scan10data = xu.io.geth5_scan(h5file,[10], "motorname1", "motorname2")
```

Reading EDF files

EDF files are mostly used to store CCD frames at ESRF recorded from various different detectors. This format is therefore used in combination with SPEC files. In an example the EDFFile class is used to parse the data from EDF files and store them to an HDF5 file. HDF5 is perfectly suited because it can handle large amount of data and compression.:

```
1 import tables
2 import xrayutilities as xu
3 import numpy
4
5 specfile = "specfile.spec"
6 h5file = "h5file.h5"
7 h5 = tables.openFile(h5file,mode='a')
8
9 s = xu.io.SPECFile(specfile,path=specdir)
10 s.Save2HDF5(h5) # save to hdf5 file
11
12 # read ccd frames from EDF files
13 for i in range(1,1000,1):
14     efile = "edfdir/sample_%04d.edf" %i
15     e = xu.io.edf.EDFFile(efile,path=specdir)
16     e.ReadData()
17     g5 = h5.createGroup(h5.root,"frelon_%04d" %i)
18     e.Save2HDF5(h5,group=g5)
19
20 h5.close()
```

See Also:

the fully working example provided in the `examples` directory perfectly suited for reading data from beamline ID01

Other formats

Other formats which can be read include

- files recorded from **Panalytical** diffractometers in the `.xrdml` format.
- files produces by the experimental control software at Hasylab/Desy (spectra).
- ccd images in the tiff file format produced by RoperScientific CCD cameras and Perkin Elmer detectors.
- files from recorded by Seifert diffractometer control software (`.nja`)
- basic support is also provided for reading of `cif` files from structure database to extract unit cell parameters

See the `examples` directory for more information and working example scripts.

4.1.2 Angle calculation using `experiment` and `material` classes

Methods for high angle x-ray diffraction experiments. Mostly for experiments performed in coplanar scattering geometry. An example will be given for the calculation of the position of Bragg reflections.

```

1 import xrayutilities as xu
2 Si = xu.materials.Si # load material from materials submodule
3
4 # initialize experimental class with directions from experiment
5 hxr = xu.HXRD(Si.Q(1,1,-2),Si.Q(1,1,1))
6 # calculate angles of Bragg reflections and print them to the screen
7 om,chi,phi,tt = hxr.Q2Ang(Si.Q(1,1,1))
8 print("Si (111)")
9 print("om,tt: %8.3f %8.3f" %(om,tt))
10 om,chi,phi,tt = hxr.Q2Ang(Si.Q(2,2,4))
11 print("Si (224)")
12 print("om,tt: %8.3f %8.3f" %(om,tt))

```

Note that on line 5 the HXRD class is initialized without specifying the energy used in the experiment. It will use the default energy stored in the configuration file, which defaults to CuK α_1 .

One could also call:

```
hxr = xu.HXRD(Si.Q(1,1,-2),Si.Q(1,1,1),en=10000) # energy in eV
```

to specify the energy explicitly. The HXRD class by default describes a four-circle goniometer as described in more detail [here](#).

Similar functions exist for other experimental geometries. For grazing incidence diffraction one might use:

```

gid = xu.GID(Si.Q(1,-1,0),Si.Q(0,0,1))
# calculate angles and print them to the screen
(alphai,azimuth,tt,beta) = gid.Q2Ang(Si.Q(2,-2,0))
print("azimuth,tt: %8.3f %8.3f" %(azimuth,tt))

```

There are two implementations for GID experiments. Both describe 2S+2D diffractometers. They differ by the order of the detector circles. One describes a setup as available at ID10B/ESRF.

There exists also a powder diffraction class, which is able to convert powder scans from angular to reciprocal space and furthermore powder scans of materials can be simulated in a very primitive way, which should only be used to get an idea of the peak positions expected from a certain material.

```

1 import xrayutilities as xu
2 import matplotlib.pyplot as plt
3
4 energy = (2*8048 + 8028)/3. # copper k alpha 1,2
5
6 # creating Indium powder
7 In_powder = xu.Powder(xu.materials.In,en=energy)
8 # calculating the reflection strength for the powder
9 In_powder.PowderIntensity()
10
11 # convoluting the peaks with a gaussian in q-space

```

```
12 peak_width = 0.01 # in q-space
13 resolution = 0.0005 # resolution in q-space
14 In_th, In_int = In_powder.Convolute(resolution, peak_width)
15
16 plt.figure()
17 plt.xlabel(r"2Theta (deg)"); plt.ylabel(r"Intensity")
18 # plot the convoluted signal
19 plt.plot(In_th*2, In_int/In_int.max(), 'k-', label="Indium powder convolution")
20 # plot each peak in a bar plot
21 plt.bar(In_powder.ang*2, In_powder.data/In_powder.data.max(), width=0.3, bottom=0,
22         linewidth=0, color='r', align='center', orientation='vertical', label="Indium bar plot")
23
24 plt.legend(); plt.set_xlim(15, 100); plt.grid()
```

One can also print the peak positions and other informations of a powder by

```
1 >>> print In_powder
2 Powder diffraction object
3 -----
4 Material: In
5 Lattice:
6 a1 = (3.252300 0.000000 0.000000), 3.252300
7 a2 = (0.000000 3.252300 0.000000), 3.252300
8 a3 = (0.000000 0.000000 4.946100), 4.946100
9 alpha = 90.000000, beta = 90.000000, gamma = 90.000000
10 Lattice base:
11 Base point 0: In (49) (0.000000 0.000000 0.000000) occ=1.00 b=0.00
12 Base point 1: In (49) (0.500000 0.500000 0.500000) occ=1.00 b=0.00
13 Reflections:
14 -----
15      h k l      |      tth      |      |Q|      |      Int      |      Int (%)
16 -----
17      [-1, 0, -1]  32.9611      2.312      217.75      100.00
18      [0, 0, -2]   36.3267      2.541      41.80       19.20
19      [-1, -1, 0]  39.1721      2.732      67.72       31.10
20      [-1, -1, -2] 54.4859      3.731      50.75       23.31
21      ....
```

4.1.3 Using the material class

xrayutilities provides a set of python classes to describe crystal lattices and materials.

Examples show how to define a new material by defining its lattice and deriving a new material, furthermore materials can be used to calculate the structure factor of a Bragg reflection for an specific energy or the energy dependency of its structure factor for anomalous scattering. Data for this are taken from a database which is included in the download.

First defining a new material from scratch is shown. This consists of an lattice with base and the type of atoms with elastic constants of the material:

```
1 import xrayutilities as xu
2
3 # defining a ZincBlendeLattice with two types of atoms and lattice constant a
4 def ZincBlendeLattice(aa, ab, a):
5     #create lattice base
6     lb = xu.materials.LatticeBase()
7     lb.append(aa, [0, 0, 0])
8     lb.append(aa, [0.5, 0.5, 0])
9     lb.append(aa, [0.5, 0, 0.5])
10    lb.append(aa, [0, 0.5, 0.5])
11    lb.append(ab, [0.25, 0.25, 0.25])
12    lb.append(ab, [0.75, 0.75, 0.25])
```

```

13     lb.append(ab, [0.75,0.25,0.75])
14     lb.append(ab, [0.25,0.75,0.75])
15
16     #create lattice vectors
17     a1 = [a,0,0]
18     a2 = [0,a,0]
19     a3 = [0,0,a]
20
21     l = xu.materials.Lattice(a1,a2,a3,base=lb)
22     return l
23
24     # defining InP, no elastic properties are given,
25     # helper functions exist to create the (6,6) elastic tensor for cubic materials
26     atom_In = xu.materials.elements.In
27     atom_P = xu.materials.elements.P
28     elastictensor = xu.materials.CubicElasticTensor(10.11e+10,5.61e+10,4.56e+10)
29     InP = xu.materials.Material("InP",ZincBlendeLattice(atom_In, atom_P ,5.8687), elastictensor)

```

InP is of course already included in the xu.materials module and can be loaded by:

```
InP = xu.materials.InP
```

like many other materials.

Using the material properties the calculation of the reflection strength of a Bragg reflection can be done as follows:

```

1  import xrayutilities as xu
2  import numpy
3
4  # defining material and experimental setup
5  InAs = xu.materials.InAs
6  energy= 8048 # eV
7
8  # calculate the structure factor for InAs (111) (222) (333)
9  hkllist = [[1,1,1],[2,2,2],[3,3,3]]
10 for hkl in hkllist:
11     qvec = InAs.Q(hkl)
12     F = InAs.StructureFactor(qvec,energy)
13     print(" |F| = %8.3f" %numpy.abs(F))

```

Similar also the energy dependence of the structure factor can be determined:

```

1  import matplotlib.pyplot as plt
2
3  energy= numpy.linspace(500,20000,5000) # 500 - 20000 eV
4  F = InAs.StructureFactorForEnergy(InAs.Q(1,1,1),energy)
5
6  plt.figure(); plt.clf()
7  plt.plot(energy,F.real,'k-',label='Re(F)')
8  plt.plot(energy,F.imag,'r-',label='Imag(F)')
9  plt.xlabel("Energy (eV)"); plt.ylabel("F"); plt.legend()

```

It is also possible to calculate the components of the structure factor of atoms, which may be needed for input into XRD simulations.:

```

1  # f = f0(|Q|) + f1(en) + j * f2(en)
2  import xrayutilities as xu
3  import numpy
4
5  Fe = xu.materials.elements.Fe # iron atom
6  Q = numpy.array([0,0,1.9],dtype=numpy.double)
7  en = 10000 # energy in eV
8
9  print "Iron (Fe): E: %9.1f eV" % en

```

```
10 print "f0: %8.4g" % Fe.f0(numpy.linalg.norm(Q))
11 print "f1: %8.4g" % Fe.f1(en)
12 print "f2: %8.4g" % Fe.f2(en)
```

4.1.4 User-specific config file

Several options of *xrayutilities* can be changed by options in a config file. This includes the default x-ray energy as well as parameters to set the number of threads used by the parallel code and the verbosity of the output.

The default options are stored inside the installed Python module and should not be changed. Instead it is suggested to use a user-specific config file ‘~/xrayutilities.conf’ or a ‘xrayutilities.conf’ file in the working directory.

An example of such a user config file is shown below:

```
# begin of xrayutilities configuration
[xrayutilities]

# verbosity level of information and debugging outputs
# 0: no output
# 1: very import notes for users
# 2: less import notes for users (e.g. intermediate results)
# 3: debugging output (e.g. print everything, which could be interesing)
# levels can be changed in the config file as well
verbosity = 1

# default wavelength in Angstrom,
wavelength = MoK $\alpha$ 1 # Molybdenum K alpha1 radiation (17479.374eV)

# default energy in eV
# if energy is given wavelength settings will be ignored
#energy = 10000 #eV

# number of threads to use in parallel sections of the code
nthreads = 1
# 0: the maximum number of available threads will be used (as returned by omp_get_max_threads())
# n: n-threads will be used
```

4.1.5 Determining detector parameters

In the following three examples of how to determine the detector parameters for linear and area detectors is given. The procedure we use is in more detail described in this [article](#).

Linear detectors

To determine the detector parameters of a linear detector one needs to perform a scan with the detector angle through the primary beam and aquire a detector spectrum at any point.

Using the following script determines the parameters necessary for the detector initialization, which are:

- pixelwidth of one channel
- the center channel
- and the detector tilt (optional)

```
1 """
2 example script to show how the detector parameters
3 such as pixel width, center channel and detector tilt
4 can be determined for a linear detector.
5 """
6
```



```

7  import xrayutilities as xu
8  import os
9
10 # load any data file with with the detector spectra of a reference scan
11 # in the primary beam, here I use spectra measured with a Seifert XRD
12 # diffractometer
13 dfile = os.path.join("data", "primarybeam_alignment20130403_2_dis350.nja")
14 s = xu.io.SeifertScan(dfile)
15
16 ang = s.axispos["T"] # detector angles during the scan
17 spectra = s.data[:, :, 1] # detector spectra aquired
18
19 # determine detector parameters
20 # this function accepts some optional arguments to describe the goniometer
21 # see the API documentation
22 pwidth, cch, tilt = xu.analysis.linear_detector_calib(ang, spectra, usetilt=True)

```

Area detector (Variant 1)

To determine the detector parameters of a area detector one needs to perform scans with the detector angles through the primary beam and aquire a detector images at any position. For the area detector at least two scans (one with the outer detector and and one with the inner detector angle) are required.

Using the following script determines the parameters necessary for the detector initialization from such scans in the primary beam only. Further down we discuss an other variant which is also able to use additionally detector images recorded at the Bragg reflection of a known reference crystal.

The determined detector parameters are:

- pixelwidth of the channels in both directions (2 parameters)
- center channels: position of the primary beam at the true zero position of the goniometer (considering the outer angle offset) (2 parameters)
- detector tilt azimuth in degree from 0 to 360
- detector tilt angle in degree (>0deg)
- detector rotation around the primary beam in degree
- outer angle offset, which describes a offset of the outer detector angle from its true zero position

The misalignment parameters can be fixed during the fitting.

```

1  """
2  example script to show the detector parameter determination for area detectors from images record
3  """
4
5  import xrayutilities as xu
6  import os
7
8  en=10300.0 #eV
9  datadir = os.path.join("data", "wire_") # data path for CCD files
10 filetmp = os.path.join(datadir, "wire_12_%05d.edf.gz") # template for the CCD file names
11
12 ## manually selected images
13 # select images which have the primary beam fully on the CCD
14 imagenrs = [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32,
15
16 images = []
17 angl = []
18 ang2 = []
19
20 # read images and angular positions from the data file

```

```
21 # this might differ for data taken at different beamlines since
22 # they way how motor positions are stored is not always consistent
23 for imgnr in imagenrs:
24     filename = filetmp%imgnr
25     edf = xu.io.EDFFile(filename)
26     images.append(edf.data)
27     ang1.append(float(edf.header['ESRF_ID01_PSIC_NANO_NU']))
28     ang2.append(float(edf.header['ESRF_ID01_PSIC_NANO_DEL']))
29
30
31 # call the fit for the detector parameters
32 # detector arm rotations and primary beam direction need to be given
33 # in total 8 parameters are fitted, however the 4 misalignment parameters can be fixed
34 # they are the detector tilt azimuth, the detector tilt angle, the detector rotation around the p
35 param,eps = xu.analysis.sample_align.area_detector_calib(ang1,ang2,images,['z+', 'y-'], 'x+', start=
```

Area detector (Variant 2)

In addition to scans in the primary beam this variant enables also the use of detector images recorded in scans at Bragg reflections of a known reference materials. However this also required that the sample orientation and x-ray wavelength need to be fit. To keep the additional parameters as small as possible we only implemented this for symmetric coplanar diffractions.

The advantage of this method is that it is more sensitive to the outer angle offset also at large detector distances. The additional parameters are:

- sample tilt angle in degree
- sample tilt azimuth in degree
- and the x-ray wavelength in Angstrom

```
1  """
2  example script to show the detector parameter determination for area detectors from images recorded
3  and at known symmetric coplanar Bragg reflections of a reference crystal
4  """
5
6  import xrayutilities as xu
7  import os
8  import numpy
9
10 Si = xu.materials.Si
11
12 datadir = 'data'
13 specfile = "si_align.spec"
14
15 en=15000 #eV
16 wl = xu.lam2en(en)
17 imgdir = os.path.join(datadir,"si_align_") # data path for CCD files
18 filetmp = "si_align_12_%04d.edf.gz"
19
20 qconv = xu.QConversion(['z+', 'y-'], ['z+', 'y-'], [1,0,0])
21 hxrd = xu.HXRD(Si.Q(1,1,-2),Si.Q(1,1,1),wl=wl,qconv=qconv)
22
23 ## manually selected images
24
25 s = xu.io.SPECFile(specfile,path=datadir)
26 for num in [61,62,63,20,21,26,27,28]:
27     s[num].ReadData()
28     try:
29         imagenrs = numpy.append(imagenrs,s[num].data['ccd_n'])
30     except:
31         imagenrs = s[num].data['ccd_n']
```

32

```

33 # avoid images which do not have to full beam on the detector as well as other which show signal
34 avoid_images = [37,57,62,63,65,87,99,106,110,111,126,130,175,181,183,185,204,206,207,208,211,212,
35
36 images = []
37 angl = [] # outer detector angle
38 ang2 = [] # inner detector angle
39 sang = [] # sample rocking angle
40 hkls = [] # Miller indices of the reference reflections
41
42 def hotpixelkill(ccd):
43     """
44     function to remove hot pixels from CCD frames
45     ADD REMOVE VALUES IF NEEDED!
46     """
47     ccd[304,97] = 0
48     ccd[303,96] = 0
49     return ccd
50
51 # read images and angular positions from the data file
52 # this might differ for data taken at different beamlines since
53 # they way how motor positions are stored is not always consistent
54 for imgnr in numpy.sort(list(set(imagenrs)-set(avoid_images))[:4]):
55     filename = os.path.join(imgdir,filetmp%imgnr)
56     edf = xu.io.EDFFile(filename)
57     ccd = hotpixelkill(edf.data)
58     images.append(ccd)
59     angl.append(float(edf.header['motor_pos'].split()[4]))
60     ang2.append(float(edf.header['motor_pos'].split()[3]))
61     sang.append(float(edf.header['motor_pos'].split()[1]))
62     if imgnr > 1293.:
63         hkls.append((0,0,0))
64     elif imgnr < 139:
65         hkls.append((0,0,numpy.sqrt(27))) # (3,3,3)
66     else:
67         hkls.append((0,0,numpy.sqrt(75))) # (5,5,5)
68
69 # call the fit for the detector parameters
70 # detector arm rotations and primary beam direction need to be given
71 # in total 8 detector parameters + 2 additional parameters for the reference crystal orientation
72 # however the 4 misalignment parameters of the detector and the 3 other parameters can be fixed
73 # the fixable parameters are detector tilt azimuth, the detector tilt angle, the detector rotation
74 # sample tilt, sample tilt azimuth and the x-ray wavelength
75 param,eps = xu.analysis.area_detector_calib_hkl(sang,ang1,ang2,images,hkls,hxrd,Si,['z+','y-'],'x')
76
77 # Following is an example of the output of the summary of the area_detector_calib_hkl function
78 #total time needed for fit: 624.51sec
79 #fitted parameters: epsilon: 9.9159e-08 (2,['Parameter convergence'])
80 #param: (cch1,cch2,pwidth1,pwidth2,tiltazimuth,tilt,detrot,outerangle_offset,sampletilt,stazimuth,
81 #param: 367.12 349.27 6.8187e-05 6.8405e-05 131.4 2.87 -0.390 -0.061 1.201 318.44 0.8254
82 #please check the resulting data (consider setting plot=True)
83 #detector rotation axis / primary beam direction (given by user): ['z+', 'y-'] / x+
84 #detector pixel directions / distance: z- y+ / 1
85 # detector initialization with: init_area('z-','y+',cch1=367.12,cch2=349.27,Nch1=516,Nch2=
86 #AND ALWAYS USE an (additional) OFFSET of -0.0611deg in the OUTER DETECTOR ANGLE!
87
88 #param,eps = xu.analysis.area_detector_calib(ang1,ang2,images,['z+','y-'],'x+',start=(45,0,0,0),f

```

4.2 xrayutilities Package

4.2.1 xrayutilities Package

xrayutilities is a Python package for assisting with x-ray diffraction experiments. Its the python package included in *xrayutilities*.

It helps with planning experiments as well as analyzing the data.

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4.2.2 config Module

module to parse xrayutilities user-specific config file the parsed values are provide as global constants for the use in other parts of xrayutilities. The config file with the default constants is found in the python installation path of xrayutilities. It is however not recommended to change things there, instead the user-specific config file ~/.xrayutilities.conf or the local xrayutilities.conf file should be used.

4.2.3 exception Module

xrayutilities derives its own exceptions which are raised upon wrong input when calling one of xrayutilities functions. none of the pre-defined exceptions is made for that purpose.

exception xrayutilities.exception.**InputError** (*msg*)

Bases: exceptions.Exception

Exception raised for errors in the input. Either wrong datatype not handled by TypeError or missing mandatory keyword argument (Note that the obligation to give keyword arguments might depend on the value of the arguments itself)

Attributes *expr* – input expression in which the error occurred :*msg*: – explanation of the error

4.2.4 experiment Module

module helping with planning and analyzing experiments

various classes are provided for

* describing experiments * calculating angular coordinates of Bragg reflections * converting angular coordinates to Q-space and vice versa * simulating powder diffraction patterns for materials

class xrayutilities.experiment.**Experiment** (*ipdir, ndir, **keyargs*)

Bases: object

base class for describing experiments users should use the derived classes: HXRD, GID, Powder

Ang2HKL (**args, **kwargs*)

angular to (h,k,l) space conversion. It will set the UB argument to Ang2Q and pass all other parameters unchanged. See Ang2Q for description of the rest of the arguments.

Parameters

****kwargs: optional keyword arguments**

B Reciprocal space conversion matrix of a Material. you can specify the matrix B (default identity matrix) shape needs to be (3,3)

mat Material object to use to obtain a B matrix (e.g. xu.materials.Si) can be used as alternative to the B keyword argument B is favored in case both are given

Uorientation matrix U can be given if none is given the orientation defined in the Experiment class is used.

dettypedetector type: one of ('point', 'linear', 'area') decides which routine of Ang2Q to call default 'point'

Returns

H K L coordinates as numpy.ndarray with shape (*, 3) where * corresponds to the number of points given in the input (*args)

Q2Ang (*qvec*)

TiltAngle (*q*, *deg=True*)

TiltAngle(*q*,*deg=True*): Return the angle between a q-space position and the surface normal.

Parameters

qlist or numpy array with the reciprocal space position

optional keyword arguments:

degTrue/False whether the return value should be in degree or radians :(default: True)

Transform (*v*)

transforms a vector, matrix or tensor of rank 4 (e.g. elasticity tensor) to the coordinate frame of the Experiment class.

Parameters

vobject to transform, list or numpy array of shape (n,) (n,n), (n,n,n,n) where n is the rank of the transformation matrix

Returns

transformed object of the same shape as v

energy

wavelength

class xrayutilities.experiment.**GID** (*idir*, *ndir*, ***keyargs*)

Bases: xrayutilities.experiment.Experiment

class describing grazing incidence x-ray diffraction experiments the class helps with calculating the angles of Bragg reflections as well as it helps with analyzing measured data

the class describes a four circle (*alpha_i*,*azimuth*,*twotheta*,*beta*) goniometer to help with GID experiments at the ROTATING ANODE. 3D data can be treated with the use of linear and area detectors. see help self.Ang2Q

Ang2Q (*ai*, *phi*, *tt*, *beta*, ***kwargs*)

angular to momentum space conversion for a point detector. Also see help GID.Ang2Q for procedures which treat line and area detectors

Parameters

ai,phi,tt,betasample and detector angles as numpy array, lists or Scalars must be given. all arguments must have the same shape or length

****kwargs: optional keyword arguments**

deltagiving delta angles to correct the given ones for misalignment delta must be an numpy array or list of length 4. used angles are than ai,phi,tt,beta - delta

Umatrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: identity matrix)

wlx-ray wavelength in angstroem (default: self._wl)

degflag to tell if angles are passed as degree (default: True)

Returns

reciprocal space positions as `numpy.ndarray` with shape `(*, 3)` where `*` corresponds to the number of points given in the input

Q2Ang (*Q*, *trans=True*, *deg=True*, ***kwargs*)

calculate the GID angles needed in the experiment the inplane reference direction defines the direction were the reference direction is parallel to the primary beam (i.e. lattice planes perpendicular to the beam)

Parameters

Q a list or numpy array of shape (3) with q-space vector components

optional keyword arguments:

trans True/False apply coordinate transformation on Q

deg True/False (default True) determines if the angles are returned in radians or degrees

Returns

a numpy array of shape (4) with the four GID scattering angles which are [alpha_i, azimuth, twotheta, beta]

alpha_i incidence angle to surface (at the moment always 0)

azimuth sample rotation with respect to the inplane reference direction

twotheta scattering angle

beta exit angle from surface (at the moment always 0)

class `xrayutilities.experiment.GID_ID10B` (*idir*, *ndir*, ***keyargs*)

Bases: `xrayutilities.experiment.GID`

class describing grazing incidence x-ray diffraction experiments the class helps with calculating the angles of Bragg reflections as well as it helps with analyzing measured data

the class describes a four circle (theta, omega, delta, gamma) goniometer to help with GID experiments at ID10B / ESRF. 3D data can be treated with the use of linear and area detectors. see help `self.Ang2Q`

Ang2Q (*th*, *om*, *delta*, *gamma*, ***kwargs*)

angular to momentum space conversion for a point detector. Also see help `GID_ID10B.Ang2Q` for procedures which treat line and area detectors

Parameters

th, om, delta, gamma sample and detector angles as numpy array, lists or Scalars must be given. all arguments must have the same shape or length

****kwargs: optional keyword arguments**

delta giving delta angles to correct the given ones for misalignment delta must be an numpy array or list of length 4. used angles are than th, om, delta, gamma - delta

UB matrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) : (default: identity matrix)

wl x-ray wavelength in angstrom (default: `self._wl`)

degflag to tell if angles are passed as degree (default: True)

Returns

reciprocal space positions as `numpy.ndarray` with shape `(*, 3)` where `*` corresponds to the number of points given in the input

Q2Ang (*Q*, *trans=True*, *deg=True*, ***kwargs*)

calculate the GID angles needed in the experiment the inplane reference direction defines the direction were the reference direction is parallel to the primary beam (i.e. lattice planes perpendicular to the beam)

Parameters

Qa list or numpy array of shape (3) with q-space vector components

optional keyword arguments:

transTrue/False apply coordinate transformation on Q

degTrue/False (default True) determines if the angles are returned in radians or degrees

Returns

a numpy array of shape (4) with the four GID scattering angles which are (theta,omega,delta,gamma)

thetaincidence angle to surface (at the moment always 0)

omegasample rotation with respect to the inplane reference direction

deltaexit angle from surface (at the moment always 0)

gammascattering angle

class xrayutilities.experiment.**GISAXS** (*idir*, *ndir*, ***keyargs*)

Bases: xrayutilities.experiment.Experiment

class describing grazing incidence x-ray diffraction experiments the class helps with calculating the angles of Bragg reflections as well as it helps with analyzing measured data

the class describes a three circle (alpha_i,twotheta,beta) goniometer to help with GISAXS experiments at the ROTATING ANODE. 3D data can be treated with the use of linear and area detectors. see help self.Ang2Q

Ang2Q (*ai*, *tt*, *beta*, ***kwargs*)

angular to momentum space conversion for a point detector. Also see help GISAXS.Ang2Q for procedures which treat line and area detectors

Parameters

ai,tt,betasample and detector angles as numpy array, lists or Scalars must be given.
all arguments must have the same shape or length

****kwargs: optional keyword arguments**

deltagiving delta angles to correct the given ones for misalignment delta must be an numpy array or list of length 3. used angles are than ai,tt,beta - delta

UBmatrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: identity matrix)

wlx-ray wavelength in angstrom (default: self._wl)

degflag to tell if angles are passed as degree (default: True)

Returns

reciprocal space positions as numpy.ndarray with shape (* , 3) where * corresponds to the number of points given in the input

Q2Ang (*Q*, *trans=True*, *deg=True*, ***kwargs*)

class xrayutilities.experiment.**HXRD** (*idir*, *ndir*, *geometry='hi_lo'*, ***keyargs*)

Bases: xrayutilities.experiment.Experiment

class describing high angle x-ray diffraction experiments the class helps with calculating the angles of Bragg reflections as well as helps with analyzing measured data

the class describes a two circle (omega,twotheta) goniometer to help with coplanar x-ray diffraction experiments. Nevertheless 3D data can be treated with the use of linear and area detectors. see help self.Ang2Q

Ang2Q (*om, tt, **kwargs*)

angular to momentum space conversion for a point detector. Also see help HXRD.Ang2Q for procedures which treat line and area detectors

Parameters

om,ttsample and detector angles as numpy array, lists or Scalars must be given. all arguments must have the same shape or length

****kwargs: optional keyword arguments**

deltagiving delta angles to correct the given ones for misalignment delta must be an numpy array or list of length 2. used angles are than om,tt - delta

UBmatrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: identity matrix)

wlx-ray wavelength in angstroem (default: self._wl)

degflag to tell if angles are passed as degree (default: True)

Returns

reciprocal space positions as numpy.ndarray with shape (*, 3) where * corresponds to the number of points given in the input

Q2Ang (**Q, **keyargs*)

Convert a reciprocal space vector Q to COPLANAR scattering angles. The keyword argument trans determines whether Q should be transformed to the experimental coordinate frame or not.

Parameters

Qa list, tuple or numpy array of shape (3) with q-space vector components or 3 separate lists with qx,qy,qz

optional keyword arguments:

transTrue/False apply coordinate transformation on Q (default True)

degTrue/Flase (default True) determines if the angles are returned in radians or degrees

geometrydetermines the scattering geometry:

- “hi_lo” high incidence and low exit

- “lo_hi” low incidence and high exit

- “real” **general geometry with angles determined by q-coordinates (azimuth); this and upper geomet**

- “realTilt” general geometry with angles determined by q-coordinates (tilt); returns [omega,chi,phi,twotheta]

defaultself.geometry

refracboolean to determine if refraction is taken into account :default: False if True then also a material must be given

matMaterial object; needed to obtain its optical properties for refraction correction, otherwise not used

full_outputboolean to determine if additional output is given to determine scattering angles more accurately in case refraction is set to True :default: False

fi,fdif refraction correction is applied one can optionally specify the facet through which the beam enters (fi) and exits (fd) fi, fd must be the surface normal vectors (not transformed & not necessarily normalized). If omitted the normal direction of the experiment is used.

Returns

a numpy array of shape (4) with four scattering angles which are [omega,chi,phi,twotheta]

omegaincidence angle with respect to surface

chisample tilt for the case of non-coplanar geometry

phisample azimuth with respect to inplane reference direction

twothetascattering angle/detector angle

if full_output: a numpy array of shape (6) with five angles which are [omega,chi,phi,twotheta,psi_i,psi_d]

psi_ioffset of the incidence beam from the scattering plane due to refraction

psi_doffset of the diffracted beam from the scattering plane due to refraction

class xrayutilities.experiment.**NonCOP** (*idir, ndir, **keyargs*)

Bases: xrayutilities.experiment.Experiment

class describing high angle x-ray diffraction experiments the class helps with calculating the angles of Bragg reflections as well as helps with analyzing measured data for NON-COPLANAR measurements, where the tilt is used to align asymmetric peaks, like in the case of a polefigure measurement.

the class describes a four circle (omega,twotheta) goniometer to help with x-ray diffraction experiments. Linear and area detectors can be treated as described in “help self.Ang2Q”

Ang2Q (*om, chi, phi, tt, **kwargs*)

angular to momentum space conversion for a point detector. Also see help NonCOP.Ang2Q for procedures which treat line and area detectors

Parameters

om,chi,phi,ttsample and detector angles as numpy array, lists or Scalars must be given. all arguments must have the same shape or length

****kwargs: optional keyword arguments**

deltagiving delta angles to correct the given ones for misalignment delta must be an numpy array or list of length 4. used angles are than om,chi,phi,tt - delta

UBmatrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: identity matrix)

wlx-ray wavelength in angstroem (default: self._wl)

degflag to tell if angles are passed as degree (default: True)

Returns

reciprocal space positions as numpy.ndarray with shape (*, 3) where * corresponds to the number of points given in the input

Q2Ang (**Q, **keyargs*)

Convert a reciprocal space vector Q to NON-COPLANAR scattering angles. The keyword argument trans determines whether Q should be transformed to the experimental coordinate frame or not.

Parameters

Qa list, tuple or numpy array of shape (3) with q-space vector components or 3 separate lists with qx,qy,qz

optional keyword arguments:

transTrue/False apply coordinate transformation on Q (default True)

degTrue/False (default True) determines if the angles are returned in radians or degree

Returns

a numpy array of shape (4) with four scattering angles which are [omega,chi,phi,twotheta]

omegasample rocking angle

chisample tilt

phisample azimuth

twothetascattering angle (detector)

class xrayutilities.experiment.**Powder** (*mat, **keyargs*)

Bases: xrayutilities.experiment.Experiment

Experimental class for powder diffraction This class is able to simulate a powder spectrum for the given material

Convolute (*stepwidth, width, min=0, max=None*)

Convolute the intensity positions with Gaussians with width in momentum space of “width”. returns array of angular positions with corresponding intensity

thetaarray with angular positions

intintensity at the positions ttheta

PowderIntensity (*tt_cutoff=180*)

Calculates the powder intensity and positions up to an angle of tt_cutoff (deg) and stores the result in:

dataarray with intensities

angangular position of intensities

qposreciprocal space position of intensities

Q2Ang (*qpos, deg=True*)

Converts reciprocal space values to theta angles

class xrayutilities.experiment.**QConversion** (*sampleAxis, detectorAxis, r_i, **kwargs*)

Bases: object

Class for the conversion of angular coordinates to momentum space for arbitrary goniometer geometries

the class is configured with the initialization and does provide three distinct routines for conversion to momentum space for

* point detector: point(...) or __call__() * linear detector: linear(...) * area detector: area(...)

linear() and area() can only be used after the init_linear() or init_area() routines were called

UB

area (**args, **kwargs*)

angular to momentum space conversion for a area detector the center pixel defined by the init_area routine must be in direction of self.r_i when detector angles are zero

the detector geometry must be initialized by the init_area(...) routine

Parameters

***args:** sample and detector angles as numpy array, lists or Scalars

in total len(self.sampleAxis)+len(detectorAxis) must be given always starting with the outer most circle all arguments must have the same shape or length

sAnglessample circle angles, number of arguments must correspond to len(self.sampleAxis)

dAnglesdetector circle angles, number of arguments must correspond to len(self.detectorAxis)

****kwargs: possible keyword arguments**

deltagiving delta angles to correct the given ones for misalignment delta must be an numpy array or list of len(*args) used angles are than *args - delta

UBmatrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: self.UB)

roiregion of interest for the detector pixels; e.g. [100,900,200,800] :(default: self._area_roi)

Navnumber of channels to average to reduce data size e.g. [2,2] :(default: self._area_nav)

wlx-ray wavelength in angstroem (default: self._wl)

degflag to tell if angles are passed as degree (default: True)

Returns

reciprocal space position of all detector pixels in a numpy.ndarray of shape ((self._area_roi[1]-self._area_roi[0]+1)*(self._area_roi[3]-self._area_roi[2]+1) , 3) were detectorDir1 is the fastest varying

detectorAxis

property handler for _detectorAxis

Returns

list of detector axis following the syntax /[xyz][+ -]/

energy

init_area(*detectorDir1, detectorDir2, cch1, cch2, Nch1, Nch2, distance=None, pwidth1=None, pwidth2=None, chpdeg1=None, chpdeg2=None, detrot=0, tiltazimuth=0, tilt=0, **kwargs*)

initialization routine for area detectors detector direction as well as distance and pixel size or channels per degree must be given. Two separate pixel sizes and channels per degree for the two orthogonal directions can be given

Parameters

detectorDir1direction of the detector (along the pixel direction 1); e.g. 'z+' means higher pixel numbers at larger z positions

detectorDir2direction of the detector (along the pixel direction 2); e.g. 'x+'

cch1,2center pixel, in direction of self.r_i at zero detectorAngles

Nch1number of detector pixels along direction 1

Nch2number of detector pixels along direction 2

distancedistance of center pixel from center of rotation

pwidth1,2width of one pixel (same unit as distance)

chpdeg1,2channels per degree (only absolute value is relevant) sign determined through detectorDir1,2

detrotangle of the detector rotation around primary beam direction (used to correct misalignments)

tiltazimuthdirection of the tilt vector in the detector plane (in degree)

tilt tilt of the detector plane around an axis normal to the direction given by the
tiltazimuth

Note: Note: Either distance and pwidth1,2 or chpdeg1,2 must be given !!

Note: Note: the channel numbers run from 0 .. NchX-1

****kwargs: optional keyword arguments**

Nav number of channels to average to reduce data size (default: [1,1])

roi region of interest for the detector pixels; e.g. [100,900,200,800]

init_linear (*detectorDir, cch, Nchannel, distance=None, pixelwidth=None, chpdeg=None, tilt=0, **kwargs*)

initialization routine for linear detectors detector direction as well as distance and pixel size or channels per degree must be given.

Parameters

detectorDir direction of the detector (along the pixel array); e.g. 'z+'

cch center channel, in direction of self.r_i at zero detectorAngles

Nchannel total number of detector channels

distance distance of center channel from center of rotation

pixelwidth width of one pixel (same unit as distance)

chpdeg channels per degree (only absolute value is relevant) sign determined through
detectorDir

!! Either distance and pixelwidth or chpdeg must be given !!

tilt tilt of the detector axis from the detectorDir (in degree)

Note: Note: the channel numbers run from 0 .. Nchannel-1

****kwargs: optional keyword arguments**

Nav number of channels to average to reduce data size (default: 1)

roi region of interest for the detector pixels; e.g. [100,900]

linear (**args, **kwargs*)

angular to momentum space conversion for a linear detector the cch of the detector must be in direction of self.r_i when detector angles are zero

the detector geometry must be initialized by the init_linear(...) routine

Parameters

***args: sample and detector angles as numpy array, lists or Scalars**

in total len(self.sampleAxis)+len(detectorAxis) must be given always starting with the
outer most circle all arguments must have the same shape or length

sAngles sample circle angles, number of arguments must correspond to
len(self.sampleAxis)

dAngles detector circle angles, number of arguments must correspond to
len(self.detectorAxis)

****kwargs: possible keyword arguments**

delta giving delta angles to correct the given ones for misalignment delta must be an numpy array or list of len(*args) used angles are than *args - delta

UB matrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: self.UB)

Nav number of channels to average to reduce data size (default: self._linear_nav)

roi region of interest for the detector pixels; e.g. [100,900] (default: self._linear_roi)

wl x-ray wavelength in angstroem (default: self._wl)

degflag to tell if angles are passed as degree (default: True)

Returns

reciprocal space position of all detector pixels in a numpy.ndarray of shape ((*)(self._linear_roi[1]-self._linear_roi[0]+1) , 3)

point (*args, **kwargs)

angular to momentum space conversion for a point detector located in direction of self.r_i when detector angles are zero

Parameters

***args: sample and detector angles as numpy array, lists**

or Scalars in total len(self.sampleAxis)+len(detectorAxis) must be given, always starting with the outer most circle. all arguments must have the same shape or length

sAngles sample circle angles, number of arguments must correspond to len(self.sampleAxis)

dAngles detector circle angles, number of arguments must correspond to len(self.detectorAxis)

****kwargs: optional keyword arguments**

delta giving delta angles to correct the given ones for misalignment delta must be an numpy array or list of len(*args) used angles are than *args - delta

UB matrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: self.UB)

wl x-ray wavelength in angstroem (default: self._wl)

degflag to tell if angles are passed as degree :(default: True)

Returns

reciprocal space positions as numpy.ndarray with shape (* , 3) where * corresponds to the number of points given in the input

sampleAxis

property handler for _sampleAxis

Returns

list of sample axis following the syntax /[xyzk][+/-]/

wavelength

4.2.5 gridder Module

class xrayutilities.gridder.**Gridder**

Bases: object

KeepData (*bool*)

Normalize (*bool*)

class xrayutilities.gridder.**Gridder1D** (*nx*)

Bases: xrayutilities.gridder.Gridder

Clear ()

data

xaxis

Returns the xaxis of the gridder the returned values correspond to the center of the data bins used by the numpy.histogram function

xrayutilities.gridder.**axis** (*min_value, max_value, n*)

Compute the a grid axis.

Parameters

Min_value axis minimum value

Max_value axis maximum value

N number of steps

xrayutilities.gridder.**check_array** (*a, dtype*)

Check if an array fits the requirements for the C-code and returns it back to the callee. Such arrays must be aligned and C_CONTIGUOUS which means that they have to follow C-ordering.

Parameters

A array to check

Dtype numpy data type

xrayutilities.gridder.**delta** (*min_value, max_value, n*)

Compute the stepsize along an axis of a grid.

Parameters

Min_value axis minimum value

Max_value axis maximum value

N number of steps

xrayutilities.gridder.**ones** (**args*)

Compute ones for matrix generation. The shape is determined by the number of input arguments.

4.2.6 gridder2d Module

class xrayutilities.gridder2d.**Gridder2D** (*nx, ny*)

Bases: xrayutilities.gridder.Gridder

Clear ()

SetResolution (*nx, ny*)

Reset the resolution of the gridder. In this case the original data stored in the object will be deleted.

Parameters

Nx number of points in x-direction

Ny number of points in y-direction

data
xaxis
xmatrix
yaxis
ymatrix

4.2.7 gridder3d Module

```
class xrayutilities.gridder3d.Gridder3D(nx, ny, nz)
    Bases: xrayutilities.gridder.Gridder
    SetResolution(nx, ny, nz)
    xaxis
    xmatrix
    yaxis
    ymatrix
    zaxis
    zmatrix
```

4.2.8 normalize Module

module to provide functions that perform block averaging of intensity arrays to reduce the amount of data (mainly for PSD and CCD measurements

and

provide functions for normalizing intensities for

* count time * absorber (user-defined function) * monitor * flatfield correction

```
class xrayutilities.normalize.IntensityNormalizer(det, **keyargs)
```

Bases: object

generic class for correction of intensity (point detector, or MCA, single CCD frames) for count time and absorber factors the class must be supplied with a absorber correction function and works with data structures provided by xrayutilities.io classes or the corresponding objects from hdf5 files read by pytables

absfun

absfun property handler returns the costum correction function or None

avmon

av_mon property handler returns the value of the average monitor or None if average is calculated from the monitor field

darkfield

flatfield property handler returns the current set darkfield of the detector or None if not set

det

det property handler returns the detector field name

flatfield

flatfield property handler returns the current set flatfield of the detector or None if not set

mon

mon property handler returns the monitor field name or None if not set

time

time property handler returns the count time or the field name of the count time or None if time is not set

`xrayutilities.normalize.blockAverage1D (data, Nav)`

perform block average for 1D array/list of Scalar values all data are used. at the end of the array a smaller cell may be used by the averaging algorithm

Parameter

datadata which should be contracted (length N)

Navnumber of values which should be averaged

Returns

block averaged numpy array of data type numpy.double (length ceil(N/Nav))

`xrayutilities.normalize.blockAverage2D (data2d, Nav1, Nav2, **kwargs)`

perform a block average for 2D array of Scalar values all data are used therefore the margin cells may differ in size

Parameter

data2darray of 2D data shape (N,M)

Nav1,Nav2a field of (Nav1 x Nav2) values is contracted

****kwargs: optional keyword argument**

roiregion of interest for the 2D array. e.g. [20,980,40,960] N = 980-20; M = 960-40

Returns

block averaged numpy array with type numpy.double with shape (ceil(N/Nav1), ceil(M/Nav2))

`xrayutilities.normalize.blockAveragePSD (psddata, Nav, **kwargs)`

perform a block average for several PSD spectra all data are used therefore the last cell used for averaging may differ in size

Parameter

psddataarray of 2D data shape (Nspectra,Nchannels)

Navnumber of channels which should be averaged

****kwargs: optional keyword argument**

roiregion of interest for the 2D array. e.g. [20,980] Nchannels = 980-20

Returns

block averaged psd spectra as numpy array with type numpy.double of shape (Nspectra , ceil(Nchannels/Nav))

4.2.9 utilities Module

xrayutilities utilities contains a conglomeration of useful functions which do not fit into one of the other files

`xrayutilities.utilities.maplog (inte, dynlow='config', dynhigh='config', **keyargs)`

clips values smaller and larger as the given bounds and returns the log10 of the input array. The bounds are given as exponent with base 10 with respect to the maximum in the input array. The function is implemented in analogy to J. Stangl's matlab implementation.

Parameters

intenumpy.array, values to be cut in range

dynlow $10^{(-dynlow)}$ will be the minimum cut off

dynhigh $10^{(-dynhigh)}$ will be the maximum cut off

optional keyword arguments (NOT IMPLEMENTED):

abslow $10^{(abslow)}$ will be taken as lower boundary

abshigh $10^{(abshigh)}$ will be taken as higher boundary

Returns

numpy.array of the same shape as inte, where values smaller/larger then $10^{(-dynlow, dynhigh)}$ were replaced by $10^{(-dynlow, dynhigh)}$

Example

```
>>> lint = maplog(int, 5, 2)
```

4.2.10 utilities_noconf Module

xrayutilities utilities contains a conglomeration of useful functions this part of utilities does not need the config class

`xrayutilities.utilities_noconf.energy(en)`

convert common energy names to energies in eV

so far this works with CuKa1, CuKa2, CuKa12, CuKb, MoKa1

Parameter

enenergy (scalar (energy in eV will be returned unchanged) or string with name of emission line)

Returns

energy in eV as float

`xrayutilities.utilities_noconf.lam2en(inp)`

converts the input energy in eV to a wavelength in Angstrom or the input wavelength in Angstrom to an energy in eV

Parameter

inpeither an energy in eV or an wavelength in Angstrom

Returns

float, energy in eV or wavlength in Angstrom

Examples

```
>>> lambda = lam2en(8048)
>>> energy = lam2en(1.5406)
```

`xrayutilities.utilities_noconf.wavelength(wl)`

convert common energy names to energies in eV

so far this works with CuKa1, CuKa2, CuKa12, CuKb, MoKa1

Parameter

wlwavelength (scalar (wavelength in Angstrom will be returned unchanged) or string with name of emission line)

Returns

wavelength in Angstrom as float

4.2.11 Subpackages

analysis Package

analysis Package

xrayutilities.analysis is a package for assisting with the analysis of x-ray diffraction data, mainly reciprocal space maps

Routines for obtaining line cuts from gridded reciprocal space maps are offered, with the ability to integrate the intensity perpendicular to the line cut direction.

line_cuts Module

`xrayutilities.analysis.line_cuts.fwhm_exp(pos, data)`

function to determine the full width at half maximum value of experimental data. Please check the obtained value visually (noise influences the result)

Parameter

pos position of the data points

data data values

Returns

fhwm value (single float)

`xrayutilities.analysis.line_cuts.get_omega_scan_ang(qx, qz, intensity, omcenter, ttcenter, omrange, npoints, **kwargs)`

extracts an omega scan from a gridded reciprocal space map

Parameters

qx equidistant array of qx momentum transfer

qz equidistant array of qz momentum transfer

intensity 2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

omcenter omega-position at which the omega scan should be extracted

ttcenter 2theta-position at which the omega scan should be extracted

omrange range of the omega scan to extract

npoints number of points of the omega scan

****kwargs**: possible keyword arguments:

qrange integration range perpendicular to scan direction

Nint number of subscans used for the integration (optionally)

lam wavelength for use in the conversion to angular coordinates

relative determines if absolute or relative omega positions are returned (default: True)

bounds flag to specify if the scan bounds should be returned (default: False)

Returns

om,omint omega scan coordinates and intensities (bounds=False)

om,omint,(qxb,qzb) omega scan coordinates and intensities + reciprocal space bounds of the extracted scan (bounds=True)

Example

```
>>> omcut, intcut = get_omega_scan(qx,qz,intensity,0.0,5.0,2.0,200)
```

```
xrayutilities.analysis.line_cuts.get_omega_scan_bounds_ang(omcenter, tt-
                                                         center, om-
                                                         range, npoints,
                                                         **kwargs)
```

return reciprocal space boundaries of omega scan

Parameters

omcenter omega-position at which the omega scan should be extracted

ttcenter 2theta-position at which the omega scan should be extracted

omrange range of the omega scan to extract

npoints number of points of the omega scan

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

lam wavelength for use in the conversion to angular coordinates

Returns

qx,qz reciprocal space coordinates of the omega scan boundaries

Example

```
>>> qxb,qzb = get_omega_scan_bounds_ang(1.0,4.0,2.4,240,qrange=0.1)
```

```
xrayutilities.analysis.line_cuts.get_omega_scan_q(qx, qz, intensity, qxcenter,
                                                  qzcenter, omrange, npoints,
                                                  **kwargs)
```

extracts an omega scan from a gridded reciprocal space map

Parameters

qx equidistant array of qx momentum transfer

qz equidistant array of qz momentum transfer

intensity 2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qxcenter qx-position at which the omega scan should be extracted

qzcenter qz-position at which the omega scan should be extracted

omrange range of the omega scan to extract

npoints number of points of the omega scan

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

Nint number of subscans used for the integration (optionally)

lam wavelength for use in the conversion to angular coordinates

relative determines if absolute or relative omega positions are returned (default: True)

bounds flag to specify if the scan bounds should be returned (default: False)

Returns

om,omint omega scan coordinates and intensities (bounds=False)

om,omint,(qxb,qzb)omega scan coordinates and intensities + reciprocal space bounds of the extracted scan (bounds=True)

Example

```
>>> omcut, intcut = get_omega_scan(qx,qz,intensity,0.0,5.0,2.0,200)
```

`xrayutilities.analysis.line_cuts.get_qx_scan(qx,qz,intensity,qzpos,**kwargs)`
extract qx line scan at position qzpos from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given range along qz

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity 2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qzpos position at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

qmin,qmax minimum and maximum value of extracted scan axis

bounds flag to specify if the scan bounds of the extracted scan should be returned (default:False)

Returns

qx,qxint qx scan coordinates and intensities (bounds=False)

qx,qxint,(qxb,qyb) qx scan coordinates and intensities + scan bounds for plotting

Example

```
>>> qxcut, qxcut_int = get_qx_scan(qx,qz,inten,5.0,qrange=0.03)
```

`xrayutilities.analysis.line_cuts.get_qz_scan(qx,qz,intensity,qxpos,**kwargs)`
extract qz line scan at position qxpos from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given range along qx

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity 2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qxpos position at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

qmin,qmax minimum and maximum value of extracted scan axis

Returns

qz,qzint qz scan coordinates and intensities

Example

```
>>> qzcut, qzcut_int = get_qz_scan(qx,qz,inten,1.5,qrange=0.03)
```

```
xrayutilities.analysis.line_cuts.get_qz_scan_int(qx, qz, intensity, qxpos,
**kwargs)
```

extracts a qz scan from a gridded reciprocal space map with integration along omega (sample rocking angle) or 2theta direction

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qxposposition at which the line scan should be extracted

****kwargs: possible keyword arguments:**

omrangeintegration range in angular direction

qmin,qmaxminimum and maximum value of extracted scan axis

boundsflag to specify if the scan bounds of the extracted scan should be returned (default:False)

intdirintegration direction 'omega': sample rocking angle (default) '2theta': scattering angle

Returns

qz,qzintqz scan coordinates and intensities (bounds=False)

qz,qzint,(qzb,qzb)qz scan coordinates and intensities + scan bounds for plotting

Example

```
>>> qzcut,qzcut_int = get_qz_scan_int(qx,qz,inten,5.0,omrange=0.3)
```

```
xrayutilities.analysis.line_cuts.get_radial_scan_ang(qx, qz, intensity, omcenter,
ttcenter, ttrange, npoints,
**kwargs)
```

extracts a radial scan from a gridded reciprocal space map

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

omcenterom-position at which the radial scan should be extracted

ttcentertt-position at which the radial scan should be extracted

ttrangetwo theta range of the radial scan to extract

npointsnumber of points of the radial scan

****kwargs: possible keyword arguments:**

omrangeintegration range perpendicular to scan direction

Nintnumber of subscans used for the integration (optionally)

lamwavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative two theta positions are returned (default=True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

om,tt,radintomega,two theta scan coordinates and intensities (bounds=False)

om,tt,radint,(qxb,qzb)radial scan coordinates and intensities + reciprocal space
bounds of the extraced scan (bounds=True)

Example

```
>>> omc,ttc,cut_int = get_radial_scan_ang(qx,qz,intensity,32.0,64.0,30.0,800,omrange=0.2)
xrayutilities.analysis.line_cuts.get_radial_scan_bounds_ang(omcenter,
                                                            ttcenter,
                                                            ttrange, npoints,
                                                            **kwargs)
```

return reciprocal space boundaries of radial scan

Parameters

omcenterom-position at which the radial scan should be extracted

ttcentertt-position at which the radial scan should be extracted

ttrangetwo theta range of the radial scan to extract

npointsnumber of points of the radial scan

****kwargs: possible keyword arguments:**

omrangeintegration range perpendicular to scan direction

lamwavelength for use in the conversion to angular coordinates

Returns

qxrad,qzradreciprocal space boundaries of radial scan

Example

```
>>>
xrayutilities.analysis.line_cuts.get_radial_scan_q(qx, qz, intensity, qxcenter,
                                                    qzcenter, ttrange, npoints,
                                                    **kwargs)
```

extracts a radial scan from a gridded reciprocal space map

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qxcenterqx-position at which the radial scan should be extracted

qzcenterqz-position at which the radial scan should be extracted

ttrangetwo theta range of the radial scan to extract

npointsnumber of points of the radial scan

****kwargs: possible keyword arguments:**

omrangeintegration range perpendicular to scan direction

Nintnumber of subscans used for the integration (optionally)

lamwavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative two theta positions are returned (default=True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

om,tt,radintomega,two theta scan coordinates and intensities (bounds=False)

om,tt,radint,(qxb,qzb)radial scan coordinates and intensities + reciprocal space bounds of the extraced scan (bounds=True)

Example

```
>>> omc,ttc,cut_int = get_radial_scan_q(qx,qz,intensity,0.0,5.0,1.0,100,omrange=0.01)
```

```
xrayutilities.analysis.line_cuts.get_ttheta_scan_ang(qx, qz, intensity, omcenter,
                                                    ttcenter, ttrange, npoints,
                                                    **kwargs)
```

extracts a twotheta scan from a gridded reciprocal space map

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

omcenterom-position at which the 2theta scan should be extracted

ttcentertt-position at which the 2theta scan should be extracted

ttrangetwo theta range of the scan to extract

npointsnumber of points of the radial scan

****kwargs: possible keyword arguments:**

omrangeintegration range in omega direction

Nintnumber of subscans used for the integration (optionally)

lamwavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative two theta positions are returned (default=True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

tt,ttinttwo theta scan coordinates and intensities (bounds=False)

tt,ttint,(qxb,qzb)2theta scan coordinates and intensities + reciprocal space bounds of the extraced scan (bounds=True)

Example

```
>>> ttc,cut_int = get_ttheta_scan_ang(qx,qz,intensity,32.0,64.0,4.0,400)
```

```
xrayutilities.analysis.line_cuts.get_ttheta_scan_bounds_ang(omcenter,
                                                            ttcenter,
                                                            ttrange, npoints,
                                                            **kwargs)
```

return reciprocal space boundaries of 2theta scan

Parameters

omcenterom-position at which the 2theta scan should be extracted

ttcentertt-position at which the 2theta scan should be extracted

ttrangetwo theta range of the 2theta scan to extract

npointsnumber of points of the 2theta scan

****kwargs: possible keyword arguments:**

omrangeintegration range in omega direction

lamwavelength for use in the conversion to angular coordinates

Returns

qxtt,qzttreciprocal space boundaries of 2theta scan (bounds=False)

tt,ttint,(qxb,qzb)2theta scan coordinates and intensities + reciprocal space bounds of the extracted scan (bounds=True)

Example

```
>>>
```

```
xrayutilities.analysis.line_cuts.get_ttheta_scan_q(qx, qz, intensity, qxcenter,
                                                    qzcenter, ttrange, npoints,
                                                    **kwargs)
```

extracts a twotheta scan from a gridded reciprocal space map

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qxcenterqx-position at which the 2theta scan should be extracted

qzcenterqz-position at which the 2theta scan should be extracted

ttrangetwo theta range of the scan to extract

npointsnumber of points of the radial scan

****kwargs**: possible keyword arguments:

omrangeintegration range in omega direction

Nintnumber of subscans used for the integration (optionally)

lamwavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative two theta positions are returned (default=True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

tt,ttinttwo theta scan coordinates and intensities (bounds=False)

om,tt,radint,(qxb,qzb)radial scan coordinates and intensities + reciprocal space bounds of the extracted scan (bounds=True)

Example

```
>>> ttc,cut_int = get_ttheta_scan_q(qx,qz,intensity,0.0,4.0,4.4,440)
```

```
xrayutilities.analysis.line_cuts.get_index(x,y,xgrid,ygrid)
```

gives the indices of the point x,y in the grid given by xgrid ygrid xgrid,ygrid must be arrays containing equidistant points

Parameters

x,ycoordinates of the point of interest (float)

xgrid,ygridgrid coordinates in x and y direction (array)

Returns

ix,iyindex of the closest gridpoint (lower left) of the point (x,y)

line_cuts3d Module

`xrayutilities.analysis.line_cuts3d.get_qx_scan3d`(*gridder*, *qypos*, *qzpos*,
***kwargs*)

extract qx line scan at position y,z from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given area around this position

Parameters

gridder3d xrayutilities.Gridder3D object containing the data

qypos,qzposposition at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrangeintegration range perpendicular to scan direction

qmin,qmaxminimum and maximum value of extracted scan axis

Returns

qx,qxintqx scan coordinates and intensities

Example

```
>>> qxcut,qxcut_int = get_qx_scan3d(gridder,0,0,qrange=0.03)
```

`xrayutilities.analysis.line_cuts3d.get_qy_scan3d`(*gridder*, *qxpos*, *qzpos*,
***kwargs*)

extract qy line scan at position x,z from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given area around this position

Parameters

gridder3d xrayutilities.Gridder3D object containing the data

qxpos,qzposposition at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrangeintegration range perpendicular to scan direction

qmin,qmaxminimum and maximum value of extracted scan axis

Returns

qy,qyintqy scan coordinates and intensities

Example

```
>>> qycut,qycut_int = get_qy_scan3d(gridder,0,0,qrange=0.03)
```

`xrayutilities.analysis.line_cuts3d.get_qz_scan3d`(*gridder*, *qxpos*, *qypos*,
***kwargs*)

extract qz line scan at position x,y from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given area around this position

Parameters

gridder3d xrayutilities.Gridder3D object containing the data

qxpos,qyposposition at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrangeintegration range perpendicular to scan direction

qmin,qmaxminimum and maximum value of extracted scan axis

Returns

qz,qzintqz scan coordinates and intensities

Example

```
>>> qzcut,qzcut_int = get_qz_scan3d(gridder,0,0,qrange=0.03)
```

`xrayutilities.analysis.line_cuts3d.get_index3d(x,y,z,xgrid,ygrid,zgrid)`

gives the indices of the point x,y,z in the grid given by xgrid ygrid zgrid xgrid,ygrid,zgrid must be arrays containing equidistant points

Parameters

x,y,zcoordinates of the point of interest (float)

xgrid,ygrid,zgridgrid coordinates in x,y,z direction (array)

Returns

ix,iy,izindex of the closest gridpoint (lower left) of the point (x,y,z)

misc Module

miscellaneous functions helpful in the analysis and experiment

`xrayutilities.analysis.misc.getangles(peak,sur,inp)`

calculates the chi and phi angles for a given peak

Parameter

peakarray which gives hkl for the peak of interest

surhkl of the surface

inpinplane reference peak or direction

Returns

[chi,phi] for the given peak on surface sur with inplane direction inp as reference

Example

```
To get the angles for the -224 peak on a 111 surface type[chi,phi] = getangles([-2,2,4],[1,1,1],[2,2,4])
```

sample_align Module

functions to help with experimental alignment during experiments, especially for experiments with linear detectors

`xrayutilities.analysis.sample_align.area_detector_calib(angle1, angle2, ccdimages, de-taxis, r_i, plot=True, cut_off=0.7, start=(0, 0, 0), fix=(False, False, False), fig=None, wl=None)`

function to calibrate the detector parameters of an area detector it determines the detector tilt possible rotations and offsets in the detector arm angles

parameters

angle1outer detector arm angle

angle2inner detector arm angle

ccdimagesimages of the ccd taken at the angles given above

detaxisdetector arm rotation axis :default: ['z+', 'y-']

r_iprimary beam direction [xyz][+-] default 'x+'

Keyword_arguments

plotflag to determine if results and intermediate results should be plotted :default: True

cut_offcut off intensity to decide if image is used for the determination or not :default: 0.7 = 70%

startsequence of start values of the fit for parameters, which can not be estimated automatically these are: tiltazimuth, tilt, detector_rotation, outerangle_offset. By default (0,0,0,0) is used.

fixfix parameters of start (default: (False,False,False,False))

figmatplotlib figure used for plotting the error :default: None (creates own figure)

wwavelength of the experiment in Angstrom (default: config.WAVELENGTH)
value does not matter here and does only affect the scaling of the error

```
xrayutilities.analysis.sample_align.area_detector_calib_hkl (sampleang,
                                                            angle1, angle2,
                                                            ccdimages, hkls,
                                                            experiment, material, detaxis,
                                                            r_i, plot=True,
                                                            cut_off=0.1,
                                                            start=(0, 0, 0,
                                                                  0, 0, 0, 'con-
fig'), fix=(False,
              False,
              False,
              False),
                                                            fig=None)
```

function to calibrate the detector parameters of an area detector it determines the detector tilt possible rotations and offsets in the detector arm angles

in this variant not only scans through the primary beam but also scans at a set of symmetric reflections can be used for the detector parameter determination. for this not only the detector parameters but in addition the sample orientation and wavelength need to be fit.

parameters

sampleangsample rocking angle (needed to align the reflections (same rotation direction as inner detector rotation)) other sample angle are not allowed to be changed during the scans

angle1outer detector arm angle

angle2inner detector arm angle

ccdimagesimages of the ccd taken at the angles given above

hklsarray/list of hkl values for every image

materialmaterial used as reference crystal

detaxisdetector arm rotation axis :default: ['z+', 'y-']

r_iprimary beam direction [xyz][+-] default 'x+'

Keyword_arguments

plotflag to determine if results and intermediate results should be plotted :default: True

cut_off cut off intensity to decide if image is used for the determination or not :default: 0.7 = 70%

start sequence of start values of the fit for parameters, which can not be estimated automatically these are: tiltazimuth, tilt, detector_rotation, outerangle_offset, stilt, stazimuth, wavelength. By default (0,0,0,0,0,0,'config') is used.

fix fix parameters of start (default: (False,False,False,False,False,False,False))

figmat plotlib figure used for plotting the error :default: None (creates own figure)

`xrayutilities.analysis.sample_align.fit_bragg_peak` (*om, tt, psd, omalign, ttalign, exphxrd, frange=(0.03, 0.03), plot=True*)

helper function to determine the Bragg peak position in a reciprocal space map used to obtain the position needed for correction of the data. the determination is done by fitting a two dimensional Gaussian (`xrayutilities.math.Gauss2d`)

PLEASE ALWAYS CHECK THE RESULT CAREFULLY!

Parameter

om,tt angular coordinates of the measurement (numpy.ndarray) either with size of psd or of psd.shape[0]

psd intensity values needed for fitting

omalign aligned omega value, used as first guess in the fit

ttalign aligned two theta values used as first guess in the fit these values are also used to set the range for the fit: the peak should be within $\pm \text{frange} \text{AA}^{-1}$ of those values

exphxrd experiment class used for the conversion between angular and reciprocal space.

frange data range used for the fit in both directions (see above for details default: (0.03,0.03) unit: AA^{-1})

plot if True (default) function will plot the result of the fit in comparison with the measurement.

Returns

Omfit, ttfit, params, covariance fitted angular values, and the fit parameters (of the Gaussian) as well as their errors

`xrayutilities.analysis.sample_align.linear_detector_calib` (*angle, mca_spectra, **keyargs*)

function to calibrate the detector distance/channel per degrees for a straight linear detector mounted on a detector arm

parameters

angle array of angles in degree of measured detector spectra

mca_spectra corresponding detector spectra :(shape: (len(angle),Nchannels))

****keyargs** passed to `psd_chdeg` function used for the modelling, additional options are:

r_iprimary beam direction as vector [xyz][+-]; default: 'y+'

detaxis detector arm rotation axis [xyz][+-] e.g. 'x+'; default: 'x+'

selected options from `psd_chdeg`:

plotflag to specify if a visualization of the fit should be done

usetilt whether to use model considering a detector tilt (deviation angle of the pixel direction from orthogonal to the primary beam) (default: True)

Note: Note: see help of `psd_chdeg` for more options

returns

pixelwidth (at one meter distance) , center_channel[, detector_tilt]

Note: Note: $L/\text{pixelwidth} \cdot \pi / 180 \sim \text{channel/degree}$, with the sample detector distance L

pixelwidth is negative in case the hit channel number decreases upon an increase of the detector angle. The function also prints out how a linear detector can be initialized using the results obtained from this calibration. Carefully check the results

`xrayutilities.analysis.sample_align.miscut_calc(phi, aomega, zeros=None, plot=True, omega0=None)`

function to calculate the miscut direction and miscut angle of a sample by fitting a sinusoidal function to the variation of the aligned omega values of more than two reflections. The function can also be used to fit reflectivity alignment values in various azimuths.

Parameters

phiazimuths in which the reflection was aligned (deg)

aomega aligned omega values (deg)

zeros(optional) angles at which surface is parallel to the beam (deg). For the analysis the angles (aomega-zeros) are used.

plotflag to specify if a visualization of the fit is wanted. :default: True

omega0 if specified the nominal value of the reflection is not included as fit parameter, but is fixed to the specified value. This value is MANDATORY if ONLY TWO AZIMUTHS are given.

Returns

[omega0, phi0, miscut]

list with fitted values for

omega0 the omega value of the reflection should be close to the nominal one

phi0 the azimuth in which the primary beam looks upstairs

miscut amplitude of the sinusoidal variation == miscut angle

`xrayutilities.analysis.sample_align.psd_chdeg(angles, channels, stdev=None, usetilt=True, plot=True, datap='kx', modelline='r-', modeltilt='b-', fignum=None, mlabel='fit', mtilt-label='fit w/tilt', dlabel='data', figtitle=True)`

function to determine the channels per degree using a linear fit of the function $nchannel = center_ch + chdeg \cdot \tan(angles)$ or the equivalent including a detector tilt

Parameters

angles detector angles for which the position of the beam was measured

channels detector channels where the beam was found

keyword arguments:

stdevstandard deviation of the beam position
plotflag to specify if a visualization of the fit should be done
usetiltwhether to use model considering a detector tilt (deviation angle of the pixel direction from orthogonal to the primary beam) (default: True)
dataplotformat of data points
modellineplotformat of modelline
modeltiltplotformat of modeltilt
fignumfigure number to use for the plot
mlabellabel of the model w/o tilt to be used in the plot
mtiltlabellabel of the model with tilt to be used in the plot
dlabellabel of the data line to be used in the plot
figtitleboolean to tell if the figure title should show the fit parameters

Returns

(pixelwidth,centerch,tilt)

Pixelwidth the width of one detector channel @ 1m distance, which is negative in case the hit channel number decreases upon an increase of the detector angle.

Centerch center channel of the detector

Tilt tilt of the detector from perpendicular to the beam (will be zero in case of usetilt=False)

Note: Note: $L/\text{pixelwidth} \cdot \pi/180 = \text{channel/degree}$ for large detector distance with the sample detector distance L

`xrayutilities.analysis.sample_align.psd_refl_align` (*primarybeam, angles, channels, plot=True*)

function which calculates the angle at which the sample is parallel to the beam from various angles and detector channels from the reflected beam. The function can be used during the half beam alignment with a linear detector.

Parameters

primarybeamprimary beam channel number
angleslist or numpy.array with angles
channelslist or numpy.array with corresponding detector channels
plotflag to specify if a visualization of the fit is wanted :default: True

Returns

omegaangle at which the sample is parallel to the beam

Example

```
>>> psd_refl_align(500, [0, 0.1, 0.2, 0.3], [550, 600, 640, 700])
```

io Package

io Package

edf Module

class xrayutilities.io.edf.**EDFDirectory** (*datapath, ext='edf', **keyargs*)

Bases: object

Parses a directory for EDF files, which can be stored to a HDF5 file for further usage

Save2HDF5 (*h5, group='', comp=True*)

Saves the data stored in the EDF files in the specified directory in a HDF5 file as a HDF5 arrays in a subgroup. By default the data is stored in a group given by the foldername - this can be changed by passing the name of a target group or a path to the target group via the “group” keyword argument.

required arguments. :h5: a HDF5 file object

optional keyword arguments: :group: group where to store the data (defaults to pathname if group is empty string) :comp: activate compression - true by default

class xrayutilities.io.edf.**EDFFile** (*fname, nxkey='Dim_1', nykey='Dim_2', dtype='DataType', path='', header=True*)

Bases: object

ReadData ()

Read the CCD data into the .data object this function is called by the initialization

Save2HDF5 (*h5, group='', comp=True*)

Saves the data stored in the EDF file in a HDF5 file as a HDF5 array. By default the data is stored in the root group of the HDF5 file - this can be changed by passing the name of a target group or a path to the target group via the “group” keyword argument.

required arguments. :h5: a HDF5 file object

optional keyword arguments: :group: group where to store the data (default to the root of the file) :comp: activate compression - true by default

imagereader Module

class xrayutilities.io.imagereader.**ImageReader** (*nop1, nop2, hdrlen=0, flatfield=None, darkfield=None, dtype=<type 'numpy.int16'>, byte_swap=False*)

Bases: object

parse CCD frames in the form of tiffs or binary data (*.bin) to numpy arrays. ignore the header since it seems to contain no useful data

The routine was tested so far withRoperScientific files with 4096x4096 pixels created at Hasylab Hamburg, which save an 16bit integer per point. Perkin Elmer images created at Hasylab Hamburg with 2048x2048 pixels.

readImage (*filename*)

read image file and correct for dark- and flatfield in case the necessary data are available.

returned data = ((image data)-(darkfield))/flatfield*average(flatfield)

Parameter

filenamefilename of the image to be read. so far only single filenames are supported.

The data might be compressed. supported extensions: .tiff, .bin and .bin.xz

class xrayutilities.io.imagereader.**PerkinElmer** (***keyargs*)

Bases: xrayutilities.io.imagereader.ImageReader

parse PerkinElmer CCD frames (*.bin) to numpy arrays Ignore the header since it seems to contain no useful data

The routine was tested only for files with 2048x2048 pixel images created at HasyLab Hamburg which save an 32bit float per point.

class xrayutilities.io.imagereader.**RoperCCD** (**keyargs)
Bases: xrayutilities.io.imagereader.ImageReader

parse RoperScientific CCD frames (*.bin) to numpy arrays Ignore the header since it seems to contain no useful data

The routine was tested only for files with 4096x4096 pixel images created at HasyLab Hamburg which save an 16bit integer per point.

panalytical_xml Module

Panalytical XML (www.XRDML.com) data file parser

based on the native python xml.dom.minidom module. want to keep the number of dependancies as small as possible

class xrayutilities.io.panalytical_xml.**XRDMLEFile** (fname)
Bases: object

class to handle XRDML data files. The class is supplied with a file name and uses the XRDMLEScan class to parse the xrdMeasurement in the file

class xrayutilities.io.panalytical_xml.**XRDMLEMeasurement** (measurement)
Bases: object

class to handle scans in a XRDML datafile

xrayutilities.io.panalytical_xml.**getOmPixel** (omraw, ttraw)

function to reshape the Omega values into a form needed for further treatment with xrayutilities

xrayutilities.io.panalytical_xml.**getxrdml_map** (filetemplate, scanrs=None, path='.',
roi=None)

parses multiple XRDML file and concatenates the results for parsing the xrayutilities.io.XRDMLEFile class is used. The function can be used for parsing maps measured with the PIXCel and point detector.

Parameter

filetemplate template string for the file names, can contain a %d which is replaced by the scan number or be a list of filenames

scanrs int or list of scan numbers

path common path to the filenames

roi region of interest for the PIXCel detector, for other measurements this is not useful!

Returns

om, tt, psd as flattened numpy arrays

Example

```
>>> om, tt, psd = xrayutilities.io.getxrdml_map("samplename_%d.xrdml", [1,2], path="./data")
```

radicon Module

python module for converting radicon data to HDF5

xrayutilities.io.radicon.**hst2hdf5** (h5, hstfile, nofchannels, h5path='/', hstpath='.')

Converts a HST file to an HDF5 file.

Required input arguments:**h5HDF5** object where to store the data**hstfilename** of the HST file**nofchannels** number of channels**optional input arguments:****h5path** Path in the HDF5 file where to store the data**hstpath** path where the HST file is located (default is the current working directory)`xrayutilities.io.radicon.rad2hdf5 (h5, rdcfile, h5path='/', rdcpath='.')`

Converts a RDC file to an HDF5 file.

Required input arguments:**h5HDF5** object where to store the data**rdcfilename** of the RDC file**optional input arguments:****h5path** Path in the HDF5 file where to store the data (default to root)**rdcpath** path where the RDC file is located (default is the current working directory)`xrayutilities.io.radicon.selecthst (et_limit, mca_info, mca_array)`

Select histograms from the complete set of recorded MCA data and stores it into a new numpy array. The selection is done due to a exposure time limit. Spectra below this limit are ignored.

required input arguments:**et_limit** exposure time limit**mca_info** pytables table with the exposure data**mca_array** array with all the MCA spectra**return value:** a numpy array with the selected mca spectra of shape (hstnr, channels).**rotanode_alignment Module**

parser for the alignment log file of the rotating anode

class `xrayutilities.io.rotanode_alignment.RA_Alignment (filename)`

Bases: object

class to parse the data file created by the alignment routine (tpalign) at the rotating anode spec installation

this routine does an iterative alignment procedure and saves the center of mass values were it moves after each scan. It iterates between two different peaks and iteratively aligns at each peak between two different motors (om/chi at symmetric peaks, om/phi at asymmetric peaks)

Parse ()

parser to read the alignment log and obtain the aligned values at every iteration.

get (key)**keys ()**

returns a list of keys for which aligned values were parsed

plot (pname)

function to plot the alignment history for a given peak

Parameters

pname peakname for which the alignment should be plotted

seifert Module

a set of routines to convert Seifert ASCII files to HDF5 in fact there exist two possibilities how the data is stored (depending on the use detector):

1. as a simple line scan (using the point detector)
2. as a map using the PSD

In the first case the data ist stored

class xrayutilities.io.seifert.**SeifertHeader**

Bases: object

save_h5_attribs (*obj*)

class xrayutilities.io.seifert.**SeifertMultiScan** (*filename, m_scan, m2, path=None*)

Bases: object

dump2hdf5 (*h5, iname='INT', group='/'*)

Saves the content of a multi-scan file to a HDF5 file. By default the data is stored in the root group of the file. To save data somewhere else the keyword argument “group” must be used.

required arguments:

h5a HDF5 file object

optional keyword arguments:

inamename for the intensity matrix

grouppath to the HDF5 group where to store the data

dump2mlab (*fname, *args*)

Store the data in a matlab file.

parse ()

class xrayutilities.io.seifert.**SeifertScan** (*filename, path=None*)

Bases: object

dump2h5 (*h5, *args, **keyargs*)

Save the data stored in the Seifert ASCII file to a HDF5 file.

required input arguments:

h5HDF5 file object

optional arguments:

names to use to store the motors. The first must be the name for the intensity array. The number of names must be equal to the second element of the shape of the data object.

optional keyword arguments:

groupHDF5 group object where to store the data.

dump2mlab (*fname, *args*)

Save the data from a Seifert scan to a matlab file.

required input arugments:

fnamename of the matlab file

optional position arguments:

names to use to store the motors. The first must be the name for the intensity array. The number of names must be equal to the second element of the shape of the data object.

parse ()

`xrayutilities.io.seifert.getSeifert_map` (*filetemplate*, *scannrs=None*, *path='.'*, *scantype='map'*, *Nchannels=1280*)

parses multiple Seifert *.nja files and concatenates the results. for parsing the `xrayutilities.io.SeifertMultiScan` class is used. The function can be used for parsing maps measured with the Meteor1D and point detector.

Parameter

filetemplate template string for the file names, can contain a %d which is replaced by the scan number or be a list of filenames

scannrs int or list of scan numbers

path common path to the filenames

scantype type of datafile: “map”: reciprocal space map measured with a regular Seifert job “tsk”: MCA spectra measured using the TaskInterpreter

Nchannels number of channels of the MCA (needed for “tsk” measurements)

Returns

om, tt, psd as flattened numpy arrays

Example

```
>>> om, tt, psd = xrayutilities.io.getSeifert_map("samplename_%d.xrdml", [1,2], path="./data")
```

`xrayutilities.io.seifert.repair_key` (*key*)

Repair a key string in the sense that the string is changed in a way that it can be used as a valid Python identifier. For that purpose all blanks within the string will be replaced by _ and leading numbers get an preceding _.

spec Module

a threaded class for observing a SPEC data file

Motivation

SPEC files can become quite large. Therefore, subsequently reading the entire file to extract a single scan is a quite cumbersome procedure. This module is a proof of concept code to write a file observer starting a reread of the file starting from a stored offset (last known scan position)

class `xrayutilities.io.spec.SPECCmdLine` (*n*, *prompt*, *cmdl*, *out*)

Bases: object

Save2HDF5 (*h5*, ***keyargs*)

class `xrayutilities.io.spec.SPECFile` (*filename*, *path=''*)

Bases: object

This class represents a single SPEC file. The class provides methodes for updateing an already opened file which makes it particular interesting for interactive use.

Parse ()

Parses the file from the starting at last_offset and adding found scans to the scan list.

Save2HDF5 (*h5f*, *comp=True*)

Save the entire file in an HDF5 file. For that purpose a group is set up in the root group of the file with the name of the file without extension and leading path. If the method is called after an previous update only the scans not written to the file meanwhile are saved.

required arguments:

h5fa HDF5 file object or its filename

optional keyword arguments:

compactivate compression - true by default

Update ()

reread the file and add newly added files. The parsing starts at the data offset of the last scan gathered during the last parsing run.

class xrayutilities.io.spec.**SPECLog** (*filename, prompt, path=''*)

Bases: object

Parse ()

Update ()

class xrayutilities.io.spec.**SPECMCA** (*nchan, roistart, roistop*)

Bases: object

SPECMCA - represents an MCA object in a SPEC file. This class is an abstract class not intended for being used directly. Instead use one of the derived classes SPECMCAFile or SPECMCAInline.

class xrayutilities.io.spec.**SPECMCAFile**

Bases: xrayutilities.io.spec.SPECMCA

ReadData ()

class xrayutilities.io.spec.**SPECMCAInline**

Bases: xrayutilities.io.spec.SPECMCA

ReadData ()

class xrayutilities.io.spec.**SPECScan** (*name, scannr, command, date, time, itime, col-names, hoffset, doffset, fid, imopnames, imopvalues, scan_status*)

Bases: object

Represents a single SPEC scan.

ClearData ()

Delete the data stored in a scan after it is no longer used.

ReadData ()

Set the data attribute of the scan class.

Save2HDF5 (*h5f, group='/', title='', desc='', optattrs={}, comp=True*)

Save a SPEC scan to an HDF5 file. The method creates a group with the name of the scan and stores the data there as a table object with name "data". By default the scan group is created under the root group of the HDF5 file. The title of the scan group is usually the scan command. Metadata of the scan are stored as attributes to the scan group. Additional custom attributes to the scan group can be passed as a dictionary via the optattrs keyword argument.

input arguments:

h5fa HDF5 file object or its filename

optional keyword arguments:

groupname or group object of the HDF5 group where to store the data

titlea string with the title for the data, defaults to the name of scan if empty

desca string with the description of the data, defaults to the scan command if empty

optattrsa dictionary with optional attributes to store for the data

compactivate compression - true by default

SetMCAParams (*mca_column_format, mca_channels, mca_start, mca_stop*)

Set the parameters used to save the MCA data to the file. This method calculates the number of lines used to store the MCA data from the number of columns and the

required input arguments:

mca_column_format number of columns used to save the data

mca_channels number of MCA channels stored

mca_start first channel that is stored

mca_stop last channel that is stored

plot (*args, **kwargs)

Plot scan data to a matplotlib figure. If newfig=True a new figure instance will be created. If logy=True (default is False) the y-axis will be plotted with a logarithmic scale.

Parameters

***args: arguments for the plot: first argument is the name of x-value column** the following pairs of arguments are the y-value names and plot styles allowed are 3,5,7,... number of arguments

****kwargs:**

newfig if True a new figure instance will be created otherwise an existing one will be used

logy if True a semilogy plot will be done

`xrayutilities.io.spec.geth5_scan(h5f, scans, *args, **kwargs)`

function to obtain the angular coordinates as well as intensity values saved in an HDF5 file, which was created from a spec file by the Save2HDF5 method. Especially usefull for reciprocal space map measurements.

further more it is possible to obtain even more positions from the data file if more than two string arguments with its names are given

Parameters

h5f file object of a HDF5 file opened using pytables or its filename

scans number of the scans of the reciprocal space map (int,tuple or list)

***args:** names of the motors (optional) (strings) to read reciprocal space maps measured in coplanar diffraction give: :omname: e.g. name of the omega motor (or its equivalent) :ttname: e.g. name of the two theta motor (or its equivalent)

****kwargs (optional):**

samplename string with the hdf5-group containing the scan data if omitted the first child node of h5f.root will be used

Returns

MAP

or

[ang1,ang2,...],MAP: angular positions of the center channel of the position sensitive detector (numpy.ndarray 1D) together with all the data values as stored in the data file (includes the intensities e.g. MAP['MCA']).

Example

```
>>> [om,tt],MAP = xu.io.geth5_scan(h5file,36,'omega','gamma')
```

spectra Module

module to handle spectra data

class `xrayutilities.io.spectra.SPECTRAFile(filename, mcatmp=None, mcastart=None, mcastop=None)`

Bases: object

Represents a SPECTRA data file. The file is read during the Constructor call. This class should work for data stored at beamlines P08 and BW2 at HASYLAB.

Required constructor arguments:

filenamea string with the name of the SPECTRA file

Optional keyword arguments:

mcatmptemplate for the MCA files

mcastart,mcastopstart and stop index for the MCA files, if not given, the class tries to determine the start and stop index automatically.

Read()

Read the data from the file.

ReadMCA()

Save2HDF5 (*h5file, name, group='/', description='SPECTRA scan', mcaname='MCA'*)

Saves the scan to an HDF5 file. The scan is saved to a separate group of name “name”. *h5file* is either a string for the file name or a HDF5 file object. If the *mca* attribute is not None *mca* data will be stored to an chunked array of with name *mcaname*.

required input arguments:

h5filestring or HDF5 file object

namename of the group where to store the data

optional keyword arguments:

grouproot group where to store the data

descriptionstring with a description of the scan

Return value: The method returns None in the case of everything went fine, True otherwise.

class xrayutilities.io.spectra.SPECTRAFileComments

Bases: dict

Class that describes the comments in the header of a SPECTRA file. The different comments are accessible via the comment keys.

class xrayutilities.io.spectra.SPECTRAFileData

Bases: object

append (*col*)

class xrayutilities.io.spectra.SPECTRAFileDataColumn (*index, name, unit, type*)

Bases: object

class xrayutilities.io.spectra.SPECTRAFileParameters

Bases: dict

class xrayutilities.io.spectra.Spectra (*data_dir*)

Bases: object

abs_corr (*data, f, **keyargs*)

Perform absorber correction. Data can be either a 1 dimensional data (point detector) or a 2D MCA array. In the case of an array the data array should be of shape (N,NChannels) where N is the number of points in the scan and NChannels the number of channels of the MCA. The absorber values are passed to the function as a 1D array of N elements.

By default the absorber values are taken from a global variable stored in the module called `_absorber_factors`. Despite this, custom values can be passed via optional keyword arguments.

required input arguments:

mcamatrix with the MCA data

ffilter values along the scan

optional keyword arguments:

ffcustom filter factors

return value:Array with the same shape as mca with the corrected MCA data.

recarray2hdf5 (*h5g, rec, name, desc*)

Save a record array in an HDF5 file. A pytables table object is used to store the data.

required input arguments:

h5gHDF5 group object or path

recrecord array

namename of the table in the file

descdescription of the table in the file

return value:

taba HDF5 table object

set_abs_factors (*ff*)

Set the global absorber factors in the module.

spectra2hdf5 (*dir, fname, mcatemp, name='', desc='SPECTRA data'*)

Convert SPECTRA scan data to a HDF5 format.

required input arguments:

dirdirectory where the scan is stored

fnamename of the SPECTRA data file

mcatemptemplate for the MCA file names

optional keyword arguments:

nameoptional name under which to save the data if empty the basename of the filename will be used

descoptional description of the scan

xrayutilities.io.spectra.get_spectra_files (*dirname*)

Return a list of spectra files within a directory.

required input arguments:

dirnamename of the directory to search

return values:list with filenames

xrayutilities.io.spectra.geth5_spectra_map (*h5file, scans, *args, **kwargs*)

function to obtain the omega and twotheta as well as intensity values for a reciprocal space map saved in an HDF5 file, which was created from a spectra file by the Save2HDF5 method.

further more it is possible to obtain even more positions from the data file if more than two string arguments with its names are given

Parameters

h5fileobject of a HDF5 file opened using pytables

scansnumber of the scans of the reciprocal space map (int,tuple or list)

***args:** arbitrary number of motor names (strings)

omnamename of the omega motor (or its equivalent)

ttnamename of the two theta motor (or its equivalent)

****kwargs** (optional):

mcaname of the mca data (if available) otherwise None (default: "MCA")

samplename string with the hdf5-group containing the scan data if omitted the first child node of h5f.root will be used to determine the sample name

Returns

[ang1,ang2,...],MAP: angular positions of the center channel of the position sensitive detector (numpy.ndarray 1D) together with all the data values as stored in the data file (includes the intensities e.g. MAP['MCA']).

`xrayutilities.io.spectra.read_data(fname)`

Read a spectra data file (a file with now MCA data).

required input arguments:

fname name of the file to read

return values: (data,hdr)

data numpy record array where the keys are the column names

hdr dictionary with header information

`xrayutilities.io.spectra.read_mca(fname)`

Read a single SPECTRA MCA file.

required input arguments:

fname name of the file to read

return value:

data a numpy array with the MCA data

`xrayutilities.io.spectra.read_mca_dir(dirname, filetemp, sort=True)`

Read all MCA files within a directory

`xrayutilities.io.spectra.read_mcas(ftemp, cntstart, cntstop)`

Read MCA data from a SPECTRA MCA directory. The filename is passed as a generic

materials Package

materials Package

`_create_database` Module

script to create the HDF5 database from the raw data of XOP this file is only needed for administration

`_create_database_alt` Module

script to create the HDF5 database from the raw data of XOP this file is only needed for administration

`cif` Module

class `xrayutilities.materials.cif.CIFFile(filename)`

Bases: `object`

class for parsing CIF (Crystallographic Information File) files. The class aims to provide an additional way of creating material classes instead of manual entering of the information the lattice constants and unit cell structure are parsed from the CIF file

Lattice ()

returns a lattice object with the structure from the CIF file

Parse ()

function to parse a CIF file. The function reads the space group symmetry operations and the basic atom positions as well as the lattice constants and unit cell angles

SymStruct ()

function to obtain the list of different atom positions in the unit cell for the different types of atoms. The data are obtained from the data parsed from the CIF file.

database Module

module to handle access to the optical parameters database

class xrayutilities.materials.database.**DataBase** (*fname*)

Bases: object

Close ()

Close an opened database file.

Create (*dbname, dbdesc*)

Creates a new database. If the database file already exists its content is delete.

required input arguments:

dbname name of the database

dbdesc a short description of the database

CreateMaterial (*name, description*)

This method creates a new material. If the material group already exists the procedure is aborted.

required input arguments:

name a string with the name of the material

description a string with a description of the material

GetF0 (*q*)

Obtain the f0 scattering factor component for a particular momentum transfer q.

required input argument:

q single float value or numpy array

GetF1 (*en*)

Return the second, energy dependent, real part of the scattering factor for a certain energy en.

required input arguments:

en float or numpy array with the energy

GetF2 (*en*)

Return the imaginary part of the scattering factor for a certain energy en.

required input arguments:

en float or numpy array with the energy

Open (*mode='r'*)

Open an existing database file.

SetF0 (*parameters*)

Save f0 fit parameters for the set material. The fit parameters are stored in the following order: c,a1,b1,.....,a4,b4

required input argument:

parameters list or numpy array with the fit parameters

SetF1 (*en, f1*)

Set f1 labels values for the active material.

required input arguments:

enlist or numpy array with energy in (eV)

f1list or numpy array with f1 values

SetF2 (*en, f2*)

Set f2 labels values for the active material.

required input arguments:

enlist or numpy array with energy in (eV)

f2list or numpy array with f2 values

SetMaterial (*name*)

Set a particular material in the database as the actual material. All operations like setting and getting optical constants are done for this particular material.

required input arguments:

namestring with the name of the material

SetWeight (*weight*)

Save weight of the element as float

required input argument:

weightatomic standard weight of the element (float)

`xrayutilities.materials.database.add_f0_from_intertab` (*db, itabfile*)

Read f0 data from international tables of crystallography and add it to the database.

`xrayutilities.materials.database.add_f0_from_xop` (*db, xopfile*)

Read f0 data from f0_xop.dat and add it to the database.

`xrayutilities.materials.database.add_f1f2_from_ascii_file` (*db, asciifile, element*)

Read f1 and f2 data for specific element from ASCII file (3 columns) and save it to the database.

`xrayutilities.materials.database.add_f1f2_from_henkedb` (*db, henkefile*)

Read f1 and f2 data from Henke database and add it to the database.

`xrayutilities.materials.database.add_f1f2_from_kissel` (*db, kisselfile*)

Read f1 and f2 data from Henke database and add it to the database.

`xrayutilities.materials.database.add_mass_from_NIST` (*db, nistfile*)

Read atoms standard mass and save it to the database.

`xrayutilities.materials.database.init_material_db` (*db*)

elements Module**lattice Module**

module handling crystal lattice structures

class `xrayutilities.materials.lattice.Atom` (*name, num*)

Bases: object

f (*q, en='config'*)

function to calculate the atomic structure factor F

Parameter

q momentum transfer

energy for which F should be calculated, if omitted the value from the xrayutilities configuration is used

Returns

f (float)

f0 (*q*)

f1 (*en*='config')

f2 (*en*='config')

xrayutilities.materials.lattice.**BCC**Lattice (*aa*, *a*)

xrayutilities.materials.lattice.**BCT**Lattice (*aa*, *a*, *c*)

xrayutilities.materials.lattice.**Baddeleyite**Lattice (*aa*, *ab*, *a*, *b*, *c*, *beta*,
deg=True)

xrayutilities.materials.lattice.**CuMnAs**Lattice (*aa*, *ab*, *ac*, *a*, *b*, *c*)

xrayutilities.materials.lattice.**CubicFm3mBaF2** (*aa*, *ab*, *a*)

xrayutilities.materials.lattice.**Cubic**Lattice (*a*)

Returns a Lattice object representing a simple cubic lattice.

required input arguments:

alattice parameter

return value:an instance of Lattice class

xrayutilities.materials.lattice.**Diamond**Lattice (*aa*, *a*)

xrayutilities.materials.lattice.**FCCL**Lattice (*aa*, *a*)

xrayutilities.materials.lattice.**GeneralPrimitive**Lattice (*a*, *b*, *c*, *alpha*, *beta*,
gamma)

xrayutilities.materials.lattice.**HCPL**Lattice (*aa*, *a*, *c*)

xrayutilities.materials.lattice.**Hexagonal3C**Lattice (*aa*, *ab*, *a*, *c*)

xrayutilities.materials.lattice.**Hexagonal4H**Lattice (*aa*, *ab*, *a*, *c*, *u*=0.1875,
v1=0.25, *v2*=0.4375)

xrayutilities.materials.lattice.**Hexagonal6H**Lattice (*aa*, *ab*, *a*, *c*)

class xrayutilities.materials.lattice.**Lattice** (*a1*, *a2*, *a3*, *base*=None)

Bases: object

class Lattice: This object represents a Bravais lattice. A lattice consists of a base

ApplyStrain (*eps*)

Applies a certain strain on a lattice. The result is a change in the base vectors.

required input arguments:

epsa 3x3 matrix independent strain components

GetPoint (**args*)

determine lattice points with indices given in the argument

Examples

```
>>> xu.materials.Si.lattice.GetPoint(0,0,4)
array([ 0.      ,  0.      , 21.72416])
```

or

```
>>> xu.materials.Si.lattice.GetPoint((1,1,1))
array([ 5.43104,  5.43104,  5.43104])
```

ReciprocalLattice()

UnitCellVolume()

function to calculate the unit cell volume of a lattice (angstrom³)

class xrayutilities.materials.lattice.**LatticeBase** (*args, **keyargs)

Bases: list

The LatticeBase class implements a container for a set of points that form the base of a crystal lattice. An instance of this class can be treated as a simple container object.

append (atom, pos, occ=1.0, b=0.0)

add new Atom to the lattice base

Parameter

atom atom object to be added

pos position of the atom

occ occupancy (default=1.0)

bb-factor of the atom used as $\exp(-b \cdot q^2 / (4 \cdot \pi)^2)$ to reduce the intensity of this atom (only used in case of temp=0 in StructureFactor and chi calculation)

xrayutilities.materials.lattice.**NaumanniteLattice** (aa, ab, a, b, c)

xrayutilities.materials.lattice.**PerovskiteTypeRhombohedral** (aa, ab, ac, a, ang)

xrayutilities.materials.lattice.**QuartzLattice** (aa, ab, a, b, c)

xrayutilities.materials.lattice.**RockSaltLattice** (aa, ab, a)

xrayutilities.materials.lattice.**RockSalt_Cubic_Lattice** (aa, ab, a)

xrayutilities.materials.lattice.**RutileLattice** (aa, ab, a, c, u)

xrayutilities.materials.lattice.**TetragonalIndiumLattice** (aa, a, c)

xrayutilities.materials.lattice.**TetragonalTinLattice** (aa, a, c)

xrayutilities.materials.lattice.**TrigonalR3mh** (aa, a, c)

xrayutilities.materials.lattice.**WurtziteLattice** (aa, ab, a, c, u=0.375, biso=0.0)

xrayutilities.materials.lattice.**ZincBlendeLattice** (aa, ab, a)

material Module

class module implements a certain material

class xrayutilities.materials.material.**Alloy** (matA, matB, x)

Bases: xrayutilities.materials.material.Material

RelaxationTriangle (hkl, sub, exp)

function which returns the relaxation triangle for a Alloy of given composition. Reciprocal space coordinates are calculated using the user-supplied experimental class

Parameter

hkl Miller Indices

sub substrate material or lattice constant (Instance of Material class or float)

exp Experiment class from which the Transformation object and ndir are needed

Returns

qy,qz reciprocal space coordinates of the corners of the relaxation triangle

lattice_const_AB (latA, latB, x)

method to set the composition of the Alloy. x is the atomic fraction of the component B

x`xrayutilities.materials.material.Cij2Cijkl (cij)`

Converts the elastic constants matrix (tensor of rank 2) to the full rank 4 cijkl tensor.

required input arguments:`cij(6,6)` cij matrix as a numpy array**return value:**`cijkl(3,3,3,3)` cijkl tensor as numpy array`xrayutilities.materials.material.Cijkl2Cij (cijkl)`

Converts the full rank 4 tensor of the elastic constants to the (6,6) matrix of elastic constants.

required input arguments:`cijkl(3,3,3,3)` cijkl tensor as numpy array**return value:**`cij(6,6)` cij matrix as a numpy array**class** `xrayutilities.materials.material.CubicAlloy (matA, matB, x)`Bases: `xrayutilities.materials.material.Alloy`**ContentBsym** (*q_inp, q_perp, hkl, sur*)

function that determines the content of B in the alloy from the reciprocal space position of an asymmetric peak and also sets the content in the current material

Parameter

q_inp inplane peak position of reflection hkl of the alloy in reciprocal space**q_perp** perpendicular peak position of the reflection hkl of the alloy in reciprocal space**hkl** Miller indices of the measured asymmetric reflection**sur** Miller indices of the surface (determines the perpendicular direction)

Returns

content, [**a_inplane**, **a_perp**, **a_bulk_perp(x)**, **eps_inplane**, **eps_perp**] : the content of B in the alloy determined from the input variables and the lattice constants calculated from the reciprocal space positions as well as the strain (eps) of the layer**ContentBsym** (*q_perp, hkl, inpr, asub, relax*)

function that determines the content of B in the alloy from the reciprocal space position of a symmetric peak. As an additional input the substrates lattice parameter and the degree of relaxation must be given

Parameter

q_perp perpendicular peak position of the reflection hkl of the alloy in reciprocal space**hkl** Miller indices of the measured symmetric reflection (also defines the surface normal)**inpr** Miller indices of a Bragg peak defining the inplane reference direction**asub** substrate lattice constant**relax** degree of relaxation (needed to obtain the content from symmetric reciprocal space position)

Returns

content the content of B in the alloy determined from the input variables

`xrayutilities.materials.material.CubicElasticTensor` (*c11, c12, c44*)

Assemble the 6x6 matrix of elastic constants for a cubic material from the three independent components of a cubic crystal

Parameter

c11,c12,c44 independent components of the elastic tensor of cubic materials

Returns

6x6 matrix with elastic constants

`xrayutilities.materials.material.GeneralUC` (*a=4, b=4, c=4, alpha=90, beta=90, gamma=90, name='General'*)

general material with primitive unit cell but possibility for different a,b,c and alpha,beta,gamma

Parameters

a,b,c unit cell extensions (Angstrom)

alpha angle between unit cell vectors b,c

beta angle between unit cell vectors a,c

gamma angle between unit cell vectors a,b

returns a Material object with the specified properties

`xrayutilities.materials.material.HexagonalElasticTensor` (*c11, c12, c13, c33, c44*)

Assemble the 6x6 matrix of elastic constants for a hexagonal material from the five independent components of a hexagonal crystal

Parameter

c11,c12,c13,c33,c44 independent components of the elastic tensor of a hexagonal material

Returns

6x6 matrix with elastic constants

class `xrayutilities.materials.material.Material` (*name, lat, cij=None, thetaDebye=None*)

Bases: object

ApplyStrain (*strain, **keyargs*)

B

GetMismatch (*mat*)

Calculate the mismatch strain between the material and a second material

Q (**hkl*)

Return the Q-space position for a certain material.

required input arguments:

hkl list or numpy array with the Miller indices (or Q(h,k,l) is also possible)

StructureFactor (*q, en='config', temp=0*)

calculates the structure factor of a material for a certain momentum transfer and energy at a certain temperature of the material

Parameter

q vectorial momentum transfer (vectors as list,tuple or numpy array are valid)

en energy in eV, if omitted the value from the xrayutilities configuration is used

temp temperature used for Debye-Waller-factor calculation

Returns

the complex structure factor

StructureFactorForEnergy (*q0, en, temp=0*)

calculates the structure factor of a material for a certain momentum transfer and a bunch of energies

Parameter

q0vectorial momentum transfer (vectors as list,tuple or numpy array are valid)

enlist, tuple or array of energy values in eV

temptemperature used for Debye-Waller-factor calculation

Returns

complex valued structure factor array

StructureFactorForQ (*q, en0='config', temp=0*)

calculates the structure factor of a material for a bunch of momentum transfers and a certain energy

Parameter

qvectorial momentum transfers; list of vectores (list, tuple or array) of length 3 e.g.:
(Si.Q(0,0,4),Si.Q(0,0,4.1),...) or numpy.array([Si.Q(0,0,4),Si.Q(0,0,4.1)])

en0energy value in eV, if omitted the value from the xrayutilities configuration is used

temptemperature used for Debye-Waller-factor calculation

Returns

complex valued structure factor array

a1

a2

a3

b1

b2

b3

beta (*en='config'*)

function to calculate the imaginary part of the deviation of the refractive index from 1 ($n=1-\delta+i\beta$)

Parameter

enx-ray energy eV, if omitted the value from the xrayutilities configuration is used

Returns

beta (float)

chi0 (*en='config'*)

calculates the complex χ_0 values often needed in simulations. They are closely related to delta and beta ($n = 1 + \chi_0/2 + i\chi''_0/2$ vs. $n = 1 - \delta + i\beta$)

chih (*q, en='config', temp=0, polarization='S'*)

calculates the complex polarizability of a material for a certain momentum transfer and energy

Parameter

qmomentum transfer in (1/Å)

enx-ray energy in eV, if omitted the value from the xrayutilities configuration is used

temptemperature used for Debye-Waller-factor calculation

polarizationeither 'S' (default) sigma or 'P' pi polarization

Returns

(abs(chih_real),abs(chih_imag)) complex polarizability

critical_angle (*en*='config', *deg*=True)

calculate critical angle for total external reflection

Parameter

enenergy of the x-rays, if omitted the value from the xrayutilities configuration is used

degreturn angle in degree if True otherwise radians (default:True)

Returns

Angle of total external reflection

dTheta (*Q*, *en*='config')

function to calculate the refractive peak shift

Parameter

Qmomentum transfer (1/Å)

enx-ray energy (eV), if omitted the value from the xrayutilities configuration is used

Returns

deltaThetapeak shift in degree

delta (*en*='config')

function to calculate the real part of the deviation of the refractive index from 1 ($n=1-\delta+i\beta$)

Parameter

enx-ray energy eV, if omitted the value from the xrayutilities configuration is used

Returns

delta (float)

idx_refraction (*en*='config')

function to calculate the complex index of refraction of a material in the x-ray range

Parameter

enenergy of the x-rays, if omitted the value from the xrayutilities configuration is used

Returns

n (complex)

lam

mu

nu

`xrayutilities.materials.material.PseudomorphicMaterial` (*submat*, *layermat*)

This function returns a material whos lattice is pseudomorphic on a particular substrate material. This function works meanwhile only for cubic materials.

required input arguments:

submatsubstrate material

layermatbulk material of the layer

return value:An instance of Material holding the new pseudomorphically strained material.

`xrayutilities.materials.material.index_map_ij2ijk1` (*ij*)

`xrayutilities.materials.material.index_map_ijk12ij` (*i*, *j*)

predefined_materials Module

class xrayutilities.materials.predefined_materials.**SiGe** (*x*)

Bases: xrayutilities.materials.material.CubicAlloy

lattice_const_AB (*latA, latB, x*)

method to calculate the lattice parameter of the SiGe alloy with composition Si_{1-x}Ge_x

x

math Package

math Package

fit Module

module with a function wrapper to scipy.optimize.leastsq for fitting of a 2D function to a peak or a 1D Gauss fit with the odr package

xrayutilities.math.fit.**fit_peak2d** (*x, y, data, start, drange, fit_function, maxfev=2000*)

fit a two dimensional function to a two dimensional data set e.g. a reciprocal space map

Parameters

x,ydata coordinates (do NOT need to be regularly spaced)

datadata set used for fitting (e.g. intensity at the data coords)

startset of starting parameters for the fit used as first parameter of function fit_function

drangelimits for the data ranges used in the fitting algorithm e.g. it is clever to use only a small region around the peak which should be fitted: [xmin,xmax,ymin,ymax]

fit_functionfunction which should be fitted must accept the parameters (x,y,*params)

Returns

(**fitparam,cov**)the set of fitted parameters and covariance matrix

xrayutilities.math.fit.**gauss_fit** (*xdata, ydata, iparams=[], maxit=200*)

Gauss fit function using odr-pack wrapper in scipy similar to :https://github.com/tiagopereira/python_tips/wiki/Scipy%3A-curve-fitting

Parameters

xdataxcoordinates of the data to be fitted

ydataycoordinates of the data which should be fit

keyword parameters:

iparamsinitial paramters for the fit (determined automatically if nothing is given)

maxitmaximal iteration number of the fit

Returns

params,sd_params,itlim

the Gauss parameters as defined in function Gauss1d(x, *param) and their errors of the fit, as well as a boolean flag which is false in the case of a successful fit

functions Module

module with several common function needed in xray data analysis

`xrayutilities.math.functions.Debye1(x)`

function to calculate the first Debye function as needed for the calculation of the thermal Debye-Waller-factor by numerical integration

for definition see: [:http://en.wikipedia.org/wiki/Debye_function](http://en.wikipedia.org/wiki/Debye_function)

$D1(x) = (1/x) \int_0^x t / (\exp(t)-1) dt$

Parameters

xargument of the Debye function (float)

Returns

D1(x)float value of the Debye function

`xrayutilities.math.functions.Gauss1d(x, *p)`

function to calculate a general one dimensional Gaussian

Parameters

plist of parameters of the Gaussian [XCEN,SIGMA,AMP,BACKGROUND] for information: SIGMA = FWHM / (2*sqrt(2*log(2)))

xcoordinate(s) where the function should be evaluated

Returns

the value of the Gaussian described by the parameters p at position x

`xrayutilities.math.functions.Gauss1d_der_p(x, *p)`

function to calculate the derivative of a Gaussian with respect the parameters p

for parameter description see Gauss1d

`xrayutilities.math.functions.Gauss1d_der_x(x, *p)`

function to calculate the derivative of a Gaussian with respect to x

for parameter description see Gauss1d

`xrayutilities.math.functions.Gauss2d(x, y, *p)`

function to calculate a general two dimensional Gaussian

Parameters

plist of parameters of the Gauss-function [XCEN,YCEN,SIGMAX,SIGMAY,AMP,BACKGROUND,ANGLE] SIGMA = FWHM / (2*sqrt(2*log(2))) ANGLE = rotation of the X,Y direction of the Gaussian in radians

x,ycoordinate(s) where the function should be evaluated

Returns

the value of the Gaussian described by the parameters p at position (x,y)

`xrayutilities.math.functions.Lorentz1d(x, *p)`

function to calculate a general one dimensional Lorentzian

Parameters

plist of parameters of the Lorentz-function [XCEN,FWHM,AMP,BACKGROUND]

x,ycoordinate(s) where the function should be evaluated

Returns

the value of the Lorentian described by the parameters p at position (x,y)

`xrayutilities.math.functions.Lorentz2d(x, y, *p)`

function to calculate a general two dimensional Lorentzian

Parameters

plist of parameters of the Lorentz-function [XCEN,YCEN,FWHMX,FWHMY,AMP,BACKGROUND,ANGLE]

ANGLE = rotation of the X,Y direction of the Lorentzian in radians

x,ycoordinate(s) where the function should be evaluated

Returns

the value of the Lorentian described by the parameters p at position (x,y)

`xrayutilities.math.functions.TwoGauss2d(x, y, *p)`

function to calculate two general two dimensional Gaussians

Parameters

plist of parameters of the Gauss-function [XCEN1,YCEN1,SIGMAX1,SIGMAY1,AMP1,ANGLE1,XCEN2,YCEN2]

SIGMA = FWHM / (2*sqrt(2*log(2))) ANGLE = rotation of the X,Y direction of

the Gaussian in radians

x,ycoordinate(s) where the function should be evaluated

Return

the value of the Gaussian described by the parameters p at position (x,y)

`xrayutilities.math.functions.kill_spike(data, threshold=2.0)`

function to smooth ****single**** data points which differ from the average of the neighboring data points by more than the threshold factor. Such spikes will be replaced by the mean value of the next neighbors.

Warning: Use this function carefully not to manipulate your data!

Parameters

data1d numpy array with experimental data

thresholdthreshold factor to identify strange data points

Returns

1d data-array with spikes removed

`xrayutilities.math.functions.smooth(x, n)`

function to smooth an array of data by averaging N adjacent data points

Parameters

x1D data array

nnumber of data points to average

Returns

xsmoothsmoothed array with same length as x

transforms Module

class `xrayutilities.math.transforms.AxisToZ(newaxis)`

Bases: `xrayutilities.math.transforms.CoordinateTransform`

Creates a coordinate transformation to move a certain axis to the z-axis. The rotation is done along the great circle. The x-axis of the new coordinate frame is created to be normal to the new and original z-axis. The new y-axis is create in order to obtain a right handed coordinate system.

`xrayutilities.math.transforms.Cij2Cijkl(cij)`

Converts the elastic constants matrix (tensor of rank 2) to the full rank 4 cijkl tensor.

required input arguments:

cij(6,6) cij matrix as a numpy array

return value:

cijkl(3,3,3,3) cijkl tensor as numpy array

`xrayutilities.math.transforms.Cijkl2Cij` (*cijkl*)

Converts the full rank 4 tensor of the elastic constants to the (6,6) matrix of elastic constants.

required input arguments:

cijkl(3,3,3,3) cijkl tensor as numpy array

return value:

cij(6,6) cij matrix as a numpy array

class `xrayutilities.math.transforms.CoordinateTransform` (*v1, v2, v3*)

Bases: `xrayutilities.math.transforms.Transform`

Create a Transformation object which transforms a point into a new coordinate frame. The new frame is determined by the three vectors *v1*/norm(*v1*), *v2*/norm(*v2*) and *v3*/norm(*v3*), which need to be orthogonal!

class `xrayutilities.math.transforms.Transform` (*matrix*)

Bases: object

inverse (**args*)

performs inverse transformation a vector, matrix or tensor of rank 4

Parameters

***args: object to transform, list or numpy array of shape(n,) (n,n), (n,n,n,n) where n is the rank of the transformation matrix**

`xrayutilities.math.transforms.XRotation` (*alpha, deg=True*)

Returns a transform that represents a rotation about the x-axis by an angle *alpha*. If *deg=True* the angle is assumed to be in degree, otherwise the function expects radians.

`xrayutilities.math.transforms.YRotation` (*alpha, deg=True*)

Returns a transform that represents a rotation about the y-axis by an angle *alpha*. If *deg=True* the angle is assumed to be in degree, otherwise the function expects radians.

`xrayutilities.math.transforms.ZRotation` (*alpha, deg=True*)

Returns a transform that represents a rotation about the z-axis by an angle *alpha*. If *deg=True* the angle is assumed to be in degree, otherwise the function expects radians.

`xrayutilities.math.transforms.index_map_ij2ijkl` (*ij*)

`xrayutilities.math.transforms.index_map_ijkl2ij` (*i, j*)

`xrayutilities.math.transforms.mycross` (*vec, mat*)

function implements the cross-product of a vector with each column of a matrix

`xrayutilities.math.transforms.rotarb` (*vec, axis, ang, deg=True*)

function implements the rotation around an arbitrary axis by an angle *ang* positive rotation is anti-clockwise when looking from positive end of axis vector

Parameter

vec numpy.array or list of length 3

axis numpy.array or list of length 3

ang rotation angle in degree (*deg=True*) or in rad (*deg=False*)

deg boolean which determines the input format of *ang* (default: True)

Returns

rotvec rotated vector as numpy.array

Example

```
>>> rotarb([1,0,0],[0,0,1],90)
array([ 6.12323400e-17,  1.00000000e+00,  0.00000000e+00])
```

`xrayutilities.math.transforms.tensorprod(vec1, vec2)`
function implements an elementwise multiplication of two vectors

vector Module

module with vector operations, mostly numpy functionality is used for the vector operation itself, however custom error checking is done to ensure vectors of length 3.

`xrayutilities.math.vector.VecAngle(v1, v2, deg=False)`
calculate the angle between two vectors. The following formula is used $v1.v2 = \text{norm}(v1)*\text{norm}(v2)*\cos(\alpha)$
 $\alpha = \arccos((v1.v2)/(\text{norm}(v1)*\text{norm}(v2)))$

required input arguments:

v1 vector as numpy array or list

v2 vector as numpy array or list

optional keyword arguments:

deg(default: false) return result in degree otherwise in radians

return value: float value with the angle inclined by the two vectors

`xrayutilities.math.vector.VecDot(v1, v2)`
Calculate the vector dot product.

required input arguments:

v1 vector as numpy array or list

v2 vector as numpy array or list

return value: float value

`xrayutilities.math.vector.VecNorm(v)`
Calculate the norm of a vector.

required input arguments:

v vector as list or numpy array

return value: float holding the vector norm

`xrayutilities.math.vector.VecUnit(v)`
Calculate the unit vector of *v*.

required input arguments:

v vector as list or numpy array

return value: numpy array with the unit vector

`xrayutilities.math.vector.getSyntax(vec)`
returns vector direction in the syntax 'x+' 'z-' or equivalents therefore works only for principle vectors of the coordinate system like e.g. [1,0,0] or [0,2,0]

Parameters

string[xyz][+-]

Returns

vector along the given direction as numpy array

`xrayutilities.math.vector.getVector (string)`

returns unit vector along a rotation axis given in the syntax 'x+' 'z-' or equivalents

Parameters

string[xyz][+-]

Returns

vector along the given direction as numpy array

4.3 analysis Package

4.3.1 analysis Package

`xrayutilities.analysis` is a package for assisting with the analysis of x-ray diffraction data, mainly reciprocal space maps

Routines for obtaining line cuts from gridded reciprocal space maps are offered, with the ability to integrate the intensity perpendicular to the line cut direction.

4.3.2 line_cuts Module

`xrayutilities.analysis.line_cuts.fwhm_exp (pos, data)`

function to determine the full width at half maximum value of experimental data. Please check the obtained value visually (noise influences the result)

Parameter

posposition of the data points

datadata values

Returns

fwhm value (single float)

`xrayutilities.analysis.line_cuts.get_omega_scan_ang (qx, qz, intensity, omcenter, ttcenter, omrange, npoints, **kwargs)`

extracts an omega scan from a gridded reciprocal space map

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

omcenteromega-position at which the omega scan should be extracted

ttcenter2theta-position at which the omega scan should be extracted

omrangerange of the omega scan to extract

npointsnumber of points of the omega scan

****kwargs**: possible keyword arguments:

qrangeintegration range perpendicular to scan direction

Nintnumber of subscans used for the integration (optionally)

lamwavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative omega positions are returned (default: True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

om,omint omega scan coordinates and intensities (bounds=False)

om,omint,(qxb,qzb) omega scan coordinates and intensities + reciprocal space bounds of the extracted scan (bounds=True)

Example

```
>>> omcut, intcut = get_omega_scan(qx,qz,intensity,0.0,5.0,2.0,200)
```

```
xrayutilities.analysis.line_cuts.get_omega_scan_bounds_ang(omcenter, tt-
                                                            center, om-
                                                            range, npoints,
                                                            **kwargs)
```

return reciprocal space boundaries of omega scan

Parameters

omcenter omega-position at which the omega scan should be extracted

ttcenter 2theta-position at which the omega scan should be extracted

omrange range of the omega scan to extract

npoints number of points of the omega scan

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

lam wavelength for use in the conversion to angular coordinates

Returns

qx,qz reciprocal space coordinates of the omega scan boundaries

Example

```
>>> qxb,qzb = get_omega_scan_bounds_ang(1.0,4.0,2.4,240,qrange=0.1)
```

```
xrayutilities.analysis.line_cuts.get_omega_scan_q(qx, qz, intensity, qxcenter,
                                                    qzcenter, omrange, npoints,
                                                    **kwargs)
```

extracts an omega scan from a gridded reciprocal space map

Parameters

qx equidistant array of qx momentum transfer

qz equidistant array of qz momentum transfer

intensity 2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qxcenter qx-position at which the omega scan should be extracted

qzcenter qz-position at which the omega scan should be extracted

omrange range of the omega scan to extract

npoints number of points of the omega scan

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

Nint number of subscans used for the integration (optionally)

lam wavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative omega positions are returned (default: True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

om,omintomega scan coordinates and intensities (bounds=False)

om,omint,(qxb,qzb)omega scan coordinates and intensities + reciprocal space bounds of the extracted scan (bounds=True)

Example

```
>>> omcut, intcut = get_omega_scan(qx,qz,intensity,0.0,5.0,2.0,200)
```

`xrayutilities.analysis.line_cuts.get_qx_scan(qx,qz,intensity,qzpos,**kwargs)`
extract qx line scan at position qzpos from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given range along qz

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity 2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qzpos position at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

qmin,qmax minimum and maximum value of extracted scan axis

boundsflag to specify if the scan bounds of the extracted scan should be returned (default:False)

Returns

qx,qxintqx scan coordinates and intensities (bounds=False)

qx,qxint,(qxb,qyb)qx scan coordinates and intensities + scan bounds for plotting

Example

```
>>> qxcut,qxcut_int = get_qx_scan(qx,qz,inten,5.0,qrange=0.03)
```

`xrayutilities.analysis.line_cuts.get_qz_scan(qx,qz,intensity,qxpos,**kwargs)`
extract qz line scan at position qxpos from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given range along qx

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity 2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qxpos position at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

qmin,qmax minimum and maximum value of extracted scan axis

Returns

qz,qzintqz scan coordinates and intensities

Example

```
>>> qzcut,qzcut_int = get_qz_scan(qx,qz,inten,1.5,qrange=0.03)
```

```
xrayutilities.analysis.line_cuts.get_qz_scan_int(qx, qz, intensity, qxpos,
**kwargs)
```

extracts a qz scan from a gridded reciprocal space map with integration along omega (sample rocking angle) or 2theta direction

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qxposposition at which the line scan should be extracted

****kwargs: possible keyword arguments:**

angrangeintegration range in angular direction

qmin,qmaxminimum and maximum value of extracted scan axis

boundsflag to specify if the scan bounds of the extracted scan should be returned (default:False)

intdirintegration direction ‘omega’: sample rocking angle (default) ‘2theta’: scattering angle

Returns

qz,qzintqz scan coordinates and intensities (bounds=False)

qz,qzint,(qzb,qzb)qz scan coordinates and intensities + scan bounds for plotting

Example

```
>>> qzcut,qzcut_int = get_qz_scan_int(qx,qz,inten,5.0,omrange=0.3)
```

```
xrayutilities.analysis.line_cuts.get_radial_scan_ang(qx, qz, intensity, omcenter,
ttcenter, ttrange, npoints,
**kwargs)
```

extracts a radial scan from a gridded reciprocal space map

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

omcenterom-position at which the radial scan should be extracted

ttcentertt-position at which the radial scan should be extracted

ttrangetwo theta range of the radial scan to extract

npointsnumber of points of the radial scan

****kwargs: possible keyword arguments:**

omrangeintegration range perpendicular to scan direction

Nintnumber of subscans used for the integration (optionally)

lamwavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative two theta positions are returned (default=True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

om,tt,radintomega,two theta scan coordinates and intensities (bounds=False)
om,tt,radint,(qxb,qzb)radial scan coordinates and intensities + reciprocal space
bounds of the extracted scan (bounds=True)

Example

```
>>> omc,ttc,cut_int = get_radial_scan_ang(qx,qz,intensity,32.0,64.0,30.0,800,omrange=0.2)

xrayutilities.analysis.line_cuts.get_radial_scan_bounds_ang(omcenter,
                                                            ttcenter,
                                                            ttrange, npoints,
                                                            **kwargs)
```

return reciprocal space boundaries of radial scan

Parameters

omcenterom-position at which the radial scan should be extracted
ttcentertt-position at which the radial scan should be extracted
ttrangetwo theta range of the radial scan to extract
npointsnumber of points of the radial scan

****kwargs: possible keyword arguments:**

omrangeintegration range perpendicular to scan direction
lamwavelength for use in the conversion to angular coordinates

Returns

qxrad,qzradreciprocal space boundaries of radial scan

Example

```
>>>

xrayutilities.analysis.line_cuts.get_radial_scan_q(qx, qz, intensity, qxcenter,
                                                    qzcenter, ttrange, npoints,
                                                    **kwargs)
```

extracts a radial scan from a gridded reciprocal space map

Parameters

qxequidistant array of qx momentum transfer
qzequidistant array of qz momentum transfer
intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)
qxcenterqx-position at which the radial scan should be extracted
qzcenterqz-position at which the radial scan should be extracted
ttrangetwo theta range of the radial scan to extract
npointsnumber of points of the radial scan

****kwargs: possible keyword arguments:**

omrangeintegration range perpendicular to scan direction
Nintnumber of subscans used for the integration (optionally)
lamwavelength for use in the conversion to angular coordinates
relativedetermines if absolute or relative two theta positions are returned (default=True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

om,tt,radintomega,two theta scan coordinates and intensities (bounds=False)

om,tt,radint,(qxb,qzb)radial scan coordinates and intensities + reciprocal space bounds of the extraced scan (bounds=True)

Example

```
>>> omc,ttc,cut_int = get_radial_scan_q(qx,qz,intensity,0.0,5.0,1.0,100,omrange=0.01)
```

```
xrayutilities.analysis.line_cuts.get_ttheta_scan_ang(qx, qz, intensity, omcenter,
                                                    ttcenter, ttrange, npoints,
                                                    **kwargs)
```

extracts a twotheta scan from a gridded reciprocal space map

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

omcenterom-position at which the 2theta scan should be extracted

ttcentertt-position at which the 2theta scan should be extracted

ttrangetwo theta range of the scan to extract

npointsnumber of points of the radial scan

****kwargs: possible keyword arguments:**

omrangeintegration range in omega direction

Nintnumber of subscans used for the integration (optionally)

lamwavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative two theta positions are returned (default=True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

tt,ttinttwo theta scan coordinates and intensities (bounds=False)

tt,ttint,(qxb,qzb)2theta scan coordinates and intensities + reciprocal space bounds of the extraced scan (bounds=True)

Example

```
>>> ttc,cut_int = get_ttheta_scan_ang(qx,qz,intensity,32.0,64.0,4.0,400)
```

```
xrayutilities.analysis.line_cuts.get_ttheta_scan_bounds_ang(omcenter,
                                                            ttcenter,
                                                            ttrange, npoints,
                                                            **kwargs)
```

return reciprocal space boundaries of 2theta scan

Parameters

omcenterom-position at which the 2theta scan should be extracted

ttcentertt-position at which the 2theta scan should be extracted

ttrangetwo theta range of the 2theta scan to extract

npointsnumber of points of the 2theta scan

****kwargs: possible keyword arguments:**

omrangeintegration range in omega direction

lamwavelength for use in the conversion to angular coordinates

Returns

qxtt,qzttreciprocal space boundaries of 2theta scan (bounds=False)

tt,ttint,(qxb,qzb)2theta scan coordinates and intensities + reciprocal space bounds of the extraced scan (bounds=True)

Example

```
>>>
```

```
xrayutilities.analysis.line_cuts.get_ttheta_scan_q(qx, qz, intensity, qxcenter,
                                                    qzcenter, ttrange, npoints,
                                                    **kwargs)
```

extracts a twotheta scan from a gridded reciprocal space map

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qxcenterqx-position at which the 2theta scan should be extracted

qzcenterqz-position at which the 2theta scan should be extracted

ttrangetwo theta range of the scan to extract

npointsnumber of points of the radial scan

****kwargs: possible keyword arguments:**

omrangeintegration range in omega direction

Nintnumber of subscans used for the integration (optionally)

lamwavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative two theta positions are returned (default=True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

tt,ttinttwo theta scan coordinates and intensities (bounds=False)

om,tt,radint,(qxb,qzb)radial scan coordinates and intensities + reciprocal space bounds of the extraced scan (bounds=True)

Example

```
>>> ttc,cut_int = get_ttheta_scan_q(qx,qz,intensity,0.0,4.0,4.4,440)
```

```
xrayutilities.analysis.line_cuts.get_index(x,y,xgrid,ygrid)
```

gives the indices of the point x,y in the grid given by xgrid ygrid xgrid,ygrid must be arrays containing equidistant points

Parameters

x,ycoordinates of the point of interest (float)

xgrid,ygridgrid coordinates in x and y direction (array)

Returns

ix, iy index of the closest gridpoint (lower left) of the point (x,y)

4.3.3 line_cuts3d Module

`xrayutilities.analysis.line_cuts3d.get_qx_scan3d(gridder, qypos, qzpos, **kwargs)`

extract qx line scan at position y,z from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given area around this position

Parameters

gridder3d xrayutilities.Gridder3D object containing the data

qypos, qzpos position at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

qmin, qmax minimum and maximum value of extracted scan axis

Returns

qx, qxint qx scan coordinates and intensities

Example

```
>>> qxcut, qxcut_int = get_qx_scan3d(gridder, 0, 0, qrange=0.03)
```

`xrayutilities.analysis.line_cuts3d.get_qy_scan3d(gridder, qxpos, qzpos, **kwargs)`

extract qy line scan at position x,z from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given area around this position

Parameters

gridder3d xrayutilities.Gridder3D object containing the data

qxpos, qzpos position at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

qmin, qmax minimum and maximum value of extracted scan axis

Returns

qy, qyint qy scan coordinates and intensities

Example

```
>>> qycut, qycut_int = get_qy_scan3d(gridder, 0, 0, qrange=0.03)
```

`xrayutilities.analysis.line_cuts3d.get_qz_scan3d(gridder, qxpos, qypos, **kwargs)`

extract qz line scan at position x,y from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given area around this position

Parameters

gridder3d xrayutilities.Gridder3D object containing the data

qxpos, qypos position at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

qmin,qmax minimum and maximum value of extracted scan axis

Returns

qz,qzint qz scan coordinates and intensities

Example

```
>>> qzcut,qzcut_int = get_qz_scan3d(gridder,0,0,qrange=0.03)
```

`xrayutilities.analysis.line_cuts3d.get_index3d(x, y, z, xgrid, ygrid, zgrid)`
gives the indices of the point x,y,z in the grid given by xgrid ygrid zgrid xgrid,ygrid,zgrid must be arrays containing equidistant points

Parameters

x,y,z coordinates of the point of interest (float)

xgrid,ygrid,zgrid grid coordinates in x,y,z direction (array)

Returns

ix,iy,iz index of the closest gridpoint (lower left) of the point (x,y,z)

4.3.4 misc Module

miscellaneous functions helpful in the analysis and experiment

`xrayutilities.analysis.misc.getangles(peak, sur, inp)`
calculates the chi and phi angles for a given peak

Parameter

peak array which gives hkl for the peak of interest

sur hkl of the surface

inp inplane reference peak or direction

Returns

[chi,phi] for the given peak on surface sur with inplane direction inp as reference

Example

```
To get the angles for the -224 peak on a 111 surface type[chi,phi] = getangles([-2,2,4],[1,1,1],[2,2,4])
```

4.3.5 sample_align Module

functions to help with experimental alignment during experiments, especially for experiments with linear detectors

`xrayutilities.analysis.sample_align.area_detector_calib(angle1, angle2, ccdimages, de-taxis, r_i, plot=True, cut_off=0.7, start=(0, 0, 0), fix=(False, False, False), fig=None, wl=None)`

function to calibrate the detector parameters of an area detector it determines the detector tilt possible rotations and offsets in the detector arm angles

parameters

angle1 outer detector arm angle

angle2inner detector arm angle

ccdimagesimages of the ccd taken at the angles given above

detaxisdetector arm rotation axis :default: ['z+', 'y-']

r_iprimary beam direction [xyz][+-] default 'x+'

Keyword_arguments

plotflag to determine if results and intermediate results should be plotted :default: True

cut_offcut off intensity to decide if image is used for the determination or not :default: 0.7 = 70%

startsequence of start values of the fit for parameters, which can not be estimated automatically these are: tiltazimuth,tilt,detector_rotation,outerangle_offset. By default (0,0,0,0) is used.

fixfix parameters of start (default: (False,False,False,False))

figmatplotlib figure used for plotting the error :default: None (creates own figure)

wwavelength of the experiment in Angstrom (default: config.WAVELENGTH) value does not matter here and does only affect the scaling of the error

```
xrayutilities.analysis.sample_align.area_detector_calib_hkl(sampleang,
                                                             angle1, angle2,
                                                             ccdimages, hkl,
                                                             experiment, material,
                                                             detaxis,
                                                             r_i, plot=True,
                                                             cut_off=0.1,
                                                             start=(0, 0, 0,
                                                             0, 0, 0, 'con-
                                                             fig'), fix=(False,
                                                             False,
                                                             False,
                                                             False,
                                                             False,
                                                             False),
                                                             fig=None)
```

function to calibrate the detector parameters of an area detector it determines the detector tilt possible rotations and offsets in the detector arm angles

in this variant not only scans through the primary beam but also scans at a set of symmetric reflections can be used for the detector parameter determination. for this not only the detector parameters but in addition the sample orientation and wavelength need to be fit.

parameters

sampleangsample rocking angle (needed to align the reflections (same rotation direction as inner detector rotation)) other sample angle are not allowed to be changed during the scans

angle1outer detector arm angle

angle2inner detector arm angle

ccdimagesimages of the ccd taken at the angles given above

hklarray/list of hkl values for every image

materialmaterial used as reference crystal

detaxisdetector arm rotation axis :default: ['z+', 'y-']

r_iprimary beam direction [xyz][+-] default 'x+'

Keyword_arguments

plotflag to determine if results and intermediate results should be plotted :default: True

cut_offcut off intensity to decide if image is used for the determination or not :default: 0.7 = 70%

startsequence of start values of the fit for parameters, which can not be estimated automatically these are: tiltazimuth,tilt,detector_rotation,outerangle_offset,stilt,stazimuth, wavelength. By default (0,0,0,0,0,0,'config') is used.

fixfix parameters of start (default: (False,False,False,False,False,False,False))

figmatplotlib figure used for plotting the error :default: None (creates own figure)

`xrayutilities.analysis.sample_align.fit_bragg_peak` (*om, tt, psd, omalign, ttalign, exphrd, frange=(0.03, 0.03), plot=True*)

helper function to determine the Bragg peak position in a reciprocal space map used to obtain the position needed for correction of the data. the determination is done by fitting a two dimensional Gaussian (`xrayutilities.math.Gauss2d`)

PLEASE ALWAYS CHECK THE RESULT CAREFULLY!

Parameter

om,ttangular coordinates of the measurement (numpy.ndarray) either with size of psd or of psd.shape[0]

psdintensity values needed for fitting

omalignaligned omega value, used as first guess in the fit

ttalignaligned two theta values used as first guess in the fit these values are also used to set the range for the fit: the peak should be within +/-frangeAA⁻¹ of those values

exphrdexperiment class used for the conversion between angular and reciprocal space.

frangedata range used for the fit in both directions (see above for details default:(0.03,0.03) unit: AA⁻¹)

plotif True (default) function will plot the result of the fit in comparison with the measurement.

Returns

Omfit,ttfit,params,covariance fitted angular values, and the fit parameters (of the Gaussian) as well as their errors

`xrayutilities.analysis.sample_align.linear_detector_calib` (*angle, mca_spectra, **keyargs*)

function to calibrate the detector distance/channel per degrees for a straight linear detector mounted on a detector arm

parameters

anglearray of angles in degree of measured detector spectra

mca_spectracorresponding detector spectra :(shape: (len(angle),Nchannels))

****keyargs** passed to `psd_chdeg` function used for the modelling, additional options are:

r_iprimary beam direction as vector [xyz][+]; default: 'y+'

detaxisdetector arm rotation axis [xyz][+]; e.g. 'x+'; default: 'x+'

selected options from psd_chdeg:

plotflag to specify if a visualization of the fit should be done

usetilt whether to use model considering a detector tilt (deviation angle of the pixel direction from orthogonal to the primary beam) (default: True)

Note: Note: see help of psd_chdeg for more options

returns

pixelwidth (at one meter distance) , center_channel[, detector_tilt]

Note: Note: $L/\text{pixelwidth} \cdot \pi/180 \approx \text{channel/degree}$, with the sample detector distance L

pixelwidth is negative in case the hit channel number decreases upon an increase of the detector angle
The function also prints out how a linear detector can be initialized using the results obtained from this calibration. Carefully check the results

`xrayutilities.analysis.sample_align.miscut_calc(phi, aomega, zeros=None, plot=True, omega0=None)`

function to calculate the miscut direction and miscut angle of a sample by fitting a sinusoidal function to the variation of the aligned omega values of more than two reflections. The function can also be used to fit reflectivity alignment values in various azimuths.

Parameters

phiazimuths in which the reflection was aligned (deg)

aomega aligned omega values (deg)

zeros(optional) angles at which surface is parallel to the beam (deg). For the analysis the angles (aomega-zeros) are used.

plotflag to specify if a visualization of the fit is wanted. :default: True

omega0 if specified the nominal value of the reflection is not included as fit parameter, but is fixed to the specified value. This value is MANDATORY if ONLY TWO AZIMUTHS are given.

Returns

[omega0, phi0, miscut]

list with fitted values for

omega0 the omega value of the reflection should be close to the nominal one

phi0 the azimuth in which the primary beam looks upstairs

miscut amplitude of the sinusoidal variation == miscut angle

`xrayutilities.analysis.sample_align.psd_chdeg(angles, channels, stdev=None, usetilt=True, plot=True, datap='kx', modelline='r-', modeltilt='b-', fignum=None, mlabel='fit', mtilt-label='fit w/tilt', dlabel='data', figtitle=True)`

function to determine the channels per degree using a linear fit of the function $nchannel = center_ch + chdeg \cdot \tan(angles)$ or the equivalent including a detector tilt

Parameters

angles detector angles for which the position of the beam was measured

channels detector channels where the beam was found

keyword arguments:

stdev standard deviation of the beam position

plot flag to specify if a visualization of the fit should be done

usetilt whether to use model considering a detector tilt (deviation angle of the pixel direction from orthogonal to the primary beam) (default: True)

data plot format of data points

model line plot format of model line

modeltilt plot format of model tilt

fignum figure number to use for the plot

mlabel label of the model w/o tilt to be used in the plot

mtiltlabel label of the model with tilt to be used in the plot

dlabel label of the data line to be used in the plot

figtitle boolean to tell if the figure title should show the fit parameters

Returns

(pixelwidth, centerch, tilt)

Pixelwidth the width of one detector channel @ 1m distance, which is negative in case the hit channel number decreases upon an increase of the detector angle.

Centerch center channel of the detector

Tilt tilt of the detector from perpendicular to the beam (will be zero in case of usetilt=False)

Note: Note: $L/\text{pixelwidth} \cdot \pi/180 = \text{channel/degree}$ for large detector distance with the sample detector distance L

`xrayutilities.analysis.sample_align.psd_refl_align` (*primarybeam, angles, channels, plot=True*)

function which calculates the angle at which the sample is parallel to the beam from various angles and detector channels from the reflected beam. The function can be used during the half beam alignment with a linear detector.

Parameters

primarybeam primary beam channel number

angles list or numpy.array with angles

channels list or numpy.array with corresponding detector channels

plot flag to specify if a visualization of the fit is wanted :default: True

Returns

omega angle at which the sample is parallel to the beam

Example

```
>>> psd_refl_align(500, [0, 0.1, 0.2, 0.3], [550, 600, 640, 700])
```

4.4 io Package

4.4.1 io Package

4.4.2 edf Module

class xrayutilities.io.edf.**EDFDirectory** (*datapath*, *ext*='edf', ***keyargs*)

Bases: object

Parses a directory for EDF files, which can be stored to a HDF5 file for further usage

Save2HDF5 (*h5*, *group*='', *comp*=True)

Saves the data stored in the EDF files in the specified directory in a HDF5 file as a HDF5 arrays in a subgroup. By default the data is stored in a group given by the foldername - this can be changed by passing the name of a target group or a path to the target group via the “group” keyword argument.

required arguments. :h5: a HDF5 file object

optional keyword arguments: :group: group where to store the data (defaults to pathname if group is empty string) :comp: activate compression - true by default

class xrayutilities.io.edf.**EDFFile** (*fname*, *nxkey*='Dim_1', *nykey*='Dim_2',
dtkey='Data Type', *path*='', *header*=True)

Bases: object

ReadData ()

Read the CCD data into the .data object this function is called by the initialization

Save2HDF5 (*h5*, *group*='', *comp*=True)

Saves the data stored in the EDF file in a HDF5 file as a HDF5 array. By default the data is stored in the root group of the HDF5 file - this can be changed by passing the name of a target group or a path to the target group via the “group” keyword argument.

required arguments. :h5: a HDF5 file object

optional keyword arguments: :group: group where to store the data (default to the root of the file)
:comp: activate compression - true by default

4.4.3 imagereader Module

class xrayutilities.io.imagereader.**ImageReader** (*nop1*, *nop2*, *hdrlen*=0, *flatfield*=None,
darkfield=None, *dtype*=<type
'numpy.int16'>, *byte_swap*=False)

Bases: object

parse CCD frames in the form of tiffs or binary data (*.bin) to numpy arrays. ignore the header since it seems to contain no useful data

The routine was tested so far withRoperScientific files with 4096x4096 pixels created at Hasylab Hamburg, which save an 16bit integer per point. Perkin Elmer images created at Hasylab Hamburg with 2048x2048 pixels.

readImage (*filename*)

read image file and correct for dark- and flatfield in case the necessary data are available.

returned data = ((image data)-(darkfield))/flatfield*average(flatfield)

Parameter

filenamefilename of the image to be read. so far only single filenames are supported.

The data might be compressed. supported extensions: .tiff, .bin and .bin.xz

class xrayutilities.io.imagereader.**PerkinElmer** (***keyargs*)

Bases: xrayutilities.io.imagereader.ImageReader

parse PerkinElmer CCD frames (*.bin) to numpy arrays Ignore the header since it seems to contain no useful data

The routine was tested only for files with 2048x2048 pixel images created at HasyLab Hamburg which save an 32bit float per point.

class xrayutilities.io.imagereader.**RoperCCD** (**keyargs)
Bases: xrayutilities.io.imagereader.ImageReader

parse RoperScientific CCD frames (*.bin) to numpy arrays Ignore the header since it seems to contain no useful data

The routine was tested only for files with 4096x4096 pixel images created at HasyLab Hamburg which save an 16bit integer per point.

4.4.4 panalytical_xml Module

Panalytical XML (www.XRDML.com) data file parser

based on the native python xml.dom.minidom module. want to keep the number of dependancies as small as possible

class xrayutilities.io.panalytical_xml.**XRDMLEFile** (fname)
Bases: object

class to handle XRDML data files. The class is supplied with a file name and uses the XRDMLEScan class to parse the xrdMeasurement in the file

class xrayutilities.io.panalytical_xml.**XRDMLEMeasurement** (measurement)
Bases: object

class to handle scans in a XRDML datafile

xrayutilities.io.panalytical_xml.**getOmPixcel** (omraw, ttraw)

function to reshape the Omega values into a form needed for further treatment with xrayutilities

xrayutilities.io.panalytical_xml.**getxrdml_map** (filetemplate, scannrs=None, path='.',
roi=None)

parses multiple XRDML file and concatenates the results for parsing the xrayutilities.io.XRDMLEFile class is used. The function can be used for parsing maps measured with the PIXCel and point detector.

Parameter

filetemplate template string for the file names, can contain a %d which is replaced by the scan number or be a list of filenames

scannrs int or list of scan numbers

path common path to the filenames

roi region of interest for the PIXCel detector, for other measurements this is not useful!

Returns

om, tt, psd as flattened numpy arrays

Example

```
>>> om, tt, psd = xrayutilities.io.getxrdml_map("samplename_%d.xrdml", [1,2], path="./data")
```

4.4.5 radicon Module

python module for converting radicon data to HDF5

xrayutilities.io.radicon.**hst2hdf5** (h5, hstfile, nofchannels, h5path='/', hstpath='.')
Converts a HST file to an HDF5 file.

Required input arguments:**h5HDF5** object where to store the data**hstfilename** of the HST file**nofchannels** number of channels**optional input arguments:****h5path** Path in the HDF5 file where to store the data**hstpath** path where the HST file is located (default is the current working directory)`xrayutilities.io.radicon.rad2hdf5 (h5, rdcfile, h5path='/', rdcpath='.')`

Converts a RDC file to an HDF5 file.

Required input arguments:**h5HDF5** object where to store the data**rdcfilename** of the RDC file**optional input arguments:****h5path** Path in the HDF5 file where to store the data (default to root)**rdcpath** path where the RDC file is located (default is the current working directory)`xrayutilities.io.radicon.selecthst (et_limit, mca_info, mca_array)`

Select histograms from the complete set of recorded MCA data and stores it into a new numpy array. The selection is done due to a exposure time limit. Spectra below this limit are ignored.

required input arguments:**et_limit** exposure time limit**mca_info** pytables table with the exposure data**mca_array** array with all the MCA spectra**return value:** a numpy array with the selected mca spectra of shape (hstnr, channels).

4.4.6 rotanode_alignment Module

parser for the alignment log file of the rotating anode

`class xrayutilities.io.rotanode_alignment.RA_Alignment (filename)`

Bases: object

class to parse the data file created by the alignment routine (tpalign) at the rotating anode spec installation

this routine does an iterative alignment procedure and saves the center of mass values were it moves after each scan. It iterates between two different peaks and iteratively aligns at each peak between two different motors (om/chi at symmetric peaks, om/phi at asymmetric peaks)

Parse ()

parser to read the alignment log and obtain the aligned values at every iteration.

get (key)**keys ()**

returns a list of keys for which aligned values were parsed

plot (pname)

function to plot the alignment history for a given peak

Parameters

pname peakname for which the alignment should be plotted

4.4.7 seifert Module

a set of routines to convert Seifert ASCII files to HDF5 in fact there exist two possibilities how the data is stored (depending on the use detector):

1. as a simple line scan (using the point detector)
2. as a map using the PSD

In the first case the data is stored

```
class xrayutilities.io.seifert.SeifertHeader
```

Bases: object

```
save_h5_attribs (obj)
```

```
class xrayutilities.io.seifert.SeifertMultiScan (filename, m_scan, m2, path=None)
```

Bases: object

```
dump2hdf5 (h5, iname='INT', group='/')
```

Saves the content of a multi-scan file to a HDF5 file. By default the data is stored in the root group of the file. To save data somewhere else the keyword argument “group” must be used.

required arguments:

h5a HDF5 file object

optional keyword arguments:

inamename for the intensity matrix

group path to the HDF5 group where to store the data

```
dump2mlab (fname, *args)
```

Store the data in a matlab file.

```
parse ()
```

```
class xrayutilities.io.seifert.SeifertScan (filename, path=None)
```

Bases: object

```
dump2h5 (h5, *args, **keyargs)
```

Save the data stored in the Seifert ASCII file to a HDF5 file.

required input arguments:

h5 HDF5 file object

optional arguments:

names to use to store the motors. The first must be the name for the intensity array. The number of names must be equal to the second element of the shape of the data object.

optional keyword arguments:

group HDF5 group object where to store the data.

```
dump2mlab (fname, *args)
```

Save the data from a Seifert scan to a matlab file.

required input arguments:

fname name of the matlab file

optional position arguments:

names to use to store the motors. The first must be the name for the intensity array. The number of names must be equal to the second element of the shape of the data object.

```
parse ()
```

`xrayutilities.io.seifert.getSeifert_map` (*filetemplate*, *scannrs=None*, *path='.'*, *scantype='map'*, *Nchannels=1280*)

parses multiple Seifert *.nja files and concatenates the results. for parsing the `xrayutilities.io.SeifertMultiScan` class is used. The function can be used for parsing maps measured with the Meteor1D and point detector.

Parameter

filetemplate template string for the file names, can contain a %d which is replaced by the scan number or be a list of filenames

scannrs int or list of scan numbers

path common path to the filenames

scantype type of datafile: “map”: reciprocal space map measured with a regular Seifert job “tsk”: MCA spectra measured using the TaskInterpreter

Nchannels number of channels of the MCA (needed for “tsk” measurements)

Returns

om, tt, psd as flattened numpy arrays

Example

```
>>> om, tt, psd = xrayutilities.io.getSeifert_map("samplename_%d.xrdml", [1,2], path="./data")
```

`xrayutilities.io.seifert.repair_key` (*key*)

Repair a key string in the sense that the string is changed in a way that it can be used as a valid Python identifier. For that purpose all blanks within the string will be replaced by _ and leading numbers get an preceding _.

4.4.8 spec Module

a threaded class for observing a SPEC data file

Motivation

SPEC files can become quite large. Therefore, subsequently reading the entire file to extract a single scan is a quite cumbersome procedure. This module is a proof of concept code to write a file observer starting a reread of the file starting from a stored offset (last known scan position)

class `xrayutilities.io.spec.SPECCmdLine` (*n*, *prompt*, *cmdl*, *out*)

Bases: object

Save2HDF5 (*h5*, ***keyargs*)

class `xrayutilities.io.spec.SPECFile` (*filename*, *path=''*)

Bases: object

This class represents a single SPEC file. The class provides methodes for updateing an already opened file which makes it particular interesting for interactive use.

Parse ()

Parses the file from the starting at last_offset and adding found scans to the scan list.

Save2HDF5 (*h5f*, *comp=True*)

Save the entire file in an HDF5 file. For that purpose a group is set up in the root group of the file with the name of the file without extension and leading path. If the method is called after an previous update only the scans not written to the file meanwhile are saved.

required arguments:

h5fa HDF5 file object or its filename

optional keyword arguments:

compactivate compression - true by default

Update ()

reread the file and add newly added files. The parsing starts at the data offset of the last scan gathered during the last parsing run.

class xrayutilities.io.spec.**SPECLog** (*filename, prompt, path=''*)

Bases: object

Parse ()

Update ()

class xrayutilities.io.spec.**SPECMCA** (*nchan, roistart, roistop*)

Bases: object

SPECMCA - represents an MCA object in a SPEC file. This class is an abstract class not intended for being used directly. Instead use one of the derived classes SPECMCAFile or SPECMCAInline.

class xrayutilities.io.spec.**SPECMCAFile**

Bases: xrayutilities.io.spec.SPECMCA

ReadData ()

class xrayutilities.io.spec.**SPECMCAInline**

Bases: xrayutilities.io.spec.SPECMCA

ReadData ()

class xrayutilities.io.spec.**SPECScan** (*name, scannr, command, date, time, itime, col-names, hoffset, doffset, fid, imopnames, imopvalues, scan_status*)

Bases: object

Represents a single SPEC scan.

ClearData ()

Delete the data stored in a scan after it is no longer used.

ReadData ()

Set the data attribute of the scan class.

Save2HDF5 (*h5f, group='/', title='', desc='', optattrs={}, comp=True*)

Save a SPEC scan to an HDF5 file. The method creates a group with the name of the scan and stores the data there as a table object with name "data". By default the scan group is created under the root group of the HDF5 file. The title of the scan group is usually the scan command. Metadata of the scan are stored as attributes to the scan group. Additional custom attributes to the scan group can be passed as a dictionary via the optattrs keyword argument.

input arguments:

h5fa HDF5 file object or its filename

optional keyword arguments:

groupname or group object of the HDF5 group where to store the data

titlea string with the title for the data, defaults to the name of scan if empty

desca string with the description of the data, defaults to the scan command if empty

optattrsa dictionary with optional attributes to store for the data

compactivate compression - true by default

SetMCAParams (*mca_column_format, mca_channels, mca_start, mca_stop*)

Set the parameters used to save the MCA data to the file. This method calculates the number of lines used to store the MCA data from the number of columns and the

required input arguments:

mca_column_format number of columns used to save the data

mca_channels number of MCA channels stored

mca_start first channel that is stored

mca_stop last channel that is stored

plot (*args, **kwargs)

Plot scan data to a matplotlib figure. If newfig=True a new figure instance will be created. If logy=True (default is False) the y-axis will be plotted with a logarithmic scale.

Parameters

***args: arguments for the plot: first argument is the name of x-value column** the following pairs of arguments are the y-value names and plot styles allowed are 3,5,7,... number of arguments

****kwargs:**

newfig if True a new figure instance will be created otherwise an existing one will be used

logy if True a semilogy plot will be done

`xrayutilities.io.spec.geth5_scan(h5f, scans, *args, **kwargs)`

function to obtain the angular coordinates as well as intensity values saved in an HDF5 file, which was created from a spec file by the Save2HDF5 method. Especially usefull for reciprocal space map measurements.

further more it is possible to obtain even more positions from the data file if more than two string arguments with its names are given

Parameters

h5f file object of a HDF5 file opened using pytables or its filename

scans number of the scans of the reciprocal space map (int,tuple or list)

***args:** names of the motors (optional) (strings) to read reciprocal space maps measured in coplanar diffraction give: :omname: e.g. name of the omega motor (or its equivalent) :ttname: e.g. name of the two theta motor (or its equivalent)

****kwargs (optional):**

samplename string with the hdf5-group containing the scan data if omitted the first child node of h5f.root will be used

Returns

MAP

or

[ang1,ang2,...],MAP: angular positions of the center channel of the position sensitive detector (numpy.ndarray 1D) together with all the data values as stored in the data file (includes the intensities e.g. MAP['MCA']).

Example

```
>>> [om,tt],MAP = xu.io.geth5_scan(h5file,36,'omega','gamma')
```

4.4.9 spectra Module

module to handle spectra data

class xrayutilities.io.spectra.SPECTRAFile (filename, mcatmp=None, mcastart=None, mcastop=None)

Bases: object

Represents a SPECTRA data file. The file is read during the Constructor call. This class should work for data stored at beamlines P08 and BW2 at HASYLAB.

Required constructor arguments:

filenamea string with the name of the SPECTRA file

Optional keyword arguments:

mcatmptemplate for the MCA files

mcastart,mcastopstart and stop index for the MCA files, if not given, the class tries to determine the start and stop index automatically.

Read()

Read the data from the file.

ReadMCA()

Save2HDF5 (*h5file, name, group='/', description='SPECTRA scan', mcaname='MCA'*)

Saves the scan to an HDF5 file. The scan is saved to a separate group of name “name”. *h5file* is either a string for the file name or a HDF5 file object. If the *mca* attribute is not None *mca* data will be stored to an chunked array of with name *mcaname*.

required input arguments:

h5filestring or HDF5 file object

namename of the group where to store the data

optional keyword arguments:

grouproot group where to store the data

descriptionstring with a description of the scan

Return value: The method returns None in the case of everything went fine, True otherwise.

class xrayutilities.io.spectra.SPECTRAFileComments

Bases: dict

Class that describes the comments in the header of a SPECTRA file. The different comments are accessible via the comment keys.

class xrayutilities.io.spectra.SPECTRAFileData

Bases: object

append (*col*)

class xrayutilities.io.spectra.SPECTRAFileDataColumn (*index, name, unit, type*)

Bases: object

class xrayutilities.io.spectra.SPECTRAFileParameters

Bases: dict

class xrayutilities.io.spectra.Spectra (*data_dir*)

Bases: object

abs_corr (*data, f, **keyargs*)

Perform absorber correction. Data can be either a 1 dimensional data (point detector) or a 2D MCA array. In the case of an array the data array should be of shape (N,NChannels) where N is the number of points in the scan and NChannels the number of channels of the MCA. The absorber values are passed to the function as a 1D array of N elements.

By default the absorber values are taken from a global variable stored in the module called `_absorber_factors`. Despite this, custom values can be passed via optional keyword arguments.

required input arguments:

mcamatrix with the MCA data

ffilter values along the scan

optional keyword arguments:

ffcustom filter factors

return value:Array with the same shape as mca with the corrected MCA data.

recarray2hdf5 (*h5g, rec, name, desc*)

Save a record array in an HDF5 file. A pytables table object is used to store the data.

required input arguments:

h5gHDF5 group object or path

recrecord array

namename of the table in the file

descdescription of the table in the file

return value:

taba HDF5 table object

set_abs_factors (*ff*)

Set the global absorber factors in the module.

spectra2hdf5 (*dir, fname, mcatemp, name='', desc='SPECTRA data'*)

Convert SPECTRA scan data to a HDF5 format.

required input arguments:

dirdirectory where the scan is stored

fnamename of the SPECTRA data file

mcatemptemplate for the MCA file names

optional keyword arguments:

nameoptional name under which to save the data if empty the basename of the filename will be used

descoptional description of the scan

xrayutilities.io.spectra.get_spectra_files (*dirname*)

Return a list of spectra files within a directory.

required input arguments:

dirnamename of the directory to search

return values:list with filenames

xrayutilities.io.spectra.geth5_spectra_map (*h5file, scans, *args, **kwargs*)

function to obtain the omega and twotheta as well as intensity values for a reciprocal space map saved in an HDF5 file, which was created from a spectra file by the Save2HDF5 method.

further more it is possible to obtain even more positions from the data file if more than two string arguments with its names are given

Parameters

h5file object of a HDF5 file opened using pytables

scansnumber of the scans of the reciprocal space map (int,tuple or list)

***args:** arbitrary number of motor names (strings)

omname of the omega motor (or its equivalent)

ttname of the two theta motor (or its equivalent)

****kwargs** (optional):

mcaname of the mca data (if available) otherwise None (default: "MCA")

samplenamestring with the hdf5-group containing the scan data if omitted the first child node of h5f.root will be used to determine the sample name

Returns

[ang1,ang2,...],MAP:angular positions of the center channel of the position sensitive detector (numpy.ndarray 1D) together with all the data values as stored in the data file (includes the intensities e.g. MAP['MCA']).

`xrayutilities.io.spectra.read_data(fname)`

Read a spectra data file (a file with now MCA data).

required input arguments:

fnamename of the file to read

return values: (data,hdr)

datanumpy record array where the keys are the column names

hdra dictionary with header information

`xrayutilities.io.spectra.read_mca(fname)`

Read a single SPECTRA MCA file.

required input arguments:

fnamename of the file to read

return value:

dataa numpy array with the MCA data

`xrayutilities.io.spectra.read_mca_dir(dirname, filetemp, sort=True)`

Read all MCA files within a directory

`xrayutilities.io.spectra.read_mcas(ftemp, cntstart, cntstop)`

Read MCA data from a SPECTRA MCA directory. The filename is passed as a generic

4.5 materials Package

4.5.1 materials Package

4.5.2 _create_database Module

script to create the HDF5 database from the raw data of XOP this file is only needed for administration

4.5.3 _create_database_alt Module

script to create the HDF5 database from the raw data of XOP this file is only needed for administration

4.5.4 cif Module

`class xrayutilities.materials.cif.CIFFile(filename)`

Bases: object

class for parsing CIF (Crystallographic Information File) files. The class aims to provide an additional way of creating material classes instead of manual entering of the information the lattice constants and unit cell structure are parsed from the CIF file

Lattice ()

returns a lattice object with the structure from the CIF file

Parse ()

function to parse a CIF file. The function reads the space group symmetry operations and the basic atom positions as well as the lattice constants and unit cell angles

SymStruct ()

function to obtain the list of different atom positions in the unit cell for the different types of atoms. The data are obtained from the data parsed from the CIF file.

4.5.5 database Module

module to handle access to the optical parameters database

class xrayutilities.materials.database.**DataBase** (*fname*)

Bases: object

Close ()

Close an opened database file.

Create (*dbname, dbdesc*)

Creates a new database. If the database file already exists its content is delete.

required input arguments:

dbname name of the database

dbdesc a short description of the database

CreateMaterial (*name, description*)

This method creates a new material. If the material group already exists the procedure is aborted.

required input arguments:

name a string with the name of the material

description a string with a description of the material

GetF0 (*q*)

Obtain the f0 scattering factor component for a particular momentum transfer *q*.

required input argument:

q single float value or numpy array

GetF1 (*en*)

Return the second, energy dependent, real part of the scattering factor for a certain energy *en*.

required input arguments:

en float or numpy array with the energy

GetF2 (*en*)

Return the imaginary part of the scattering factor for a certain energy *en*.

required input arguments:

en float or numpy array with the energy

Open (*mode='r'*)

Open an existing database file.

SetF0 (*parameters*)

Save f0 fit parameters for the set material. The fit parameters are stored in the following order: *c, a1, b1, ..., a4, b4*

required input argument:

parameters list or numpy array with the fit parameters

SetF1 (*en, f1*)

Set f1 labels values for the active material.

required input arguments:

enlist or numpy array with energy in (eV)

f1list or numpy array with f1 values

SetF2 (*en, f2*)

Set f2 labels values for the active material.

required input arguments:

enlist or numpy array with energy in (eV)

f2list or numpy array with f2 values

SetMaterial (*name*)

Set a particular material in the database as the actual material. All operations like setting and getting optical constants are done for this particular material.

required input arguments:

namestring with the name of the material

SetWeight (*weight*)

Save weight of the element as float

required input argument:

weightatomic standard weight of the element (float)

`xrayutilities.materials.database.add_f0_from_intertab (db, itabfile)`

Read f0 data from international tables of crystallography and add it to the database.

`xrayutilities.materials.database.add_f0_from_xop (db, xopfile)`

Read f0 data from f0_xop.dat and add it to the database.

`xrayutilities.materials.database.add_f1f2_from_ascii_file (db, asciifile, element)`

Read f1 and f2 data for specific element from ASCII file (3 columns) and save it to the database.

`xrayutilities.materials.database.add_f1f2_from_henkedb (db, henkefile)`

Read f1 and f2 data from Henke database and add it to the database.

`xrayutilities.materials.database.add_f1f2_from_kissel (db, kisselfile)`

Read f1 and f2 data from Henke database and add it to the database.

`xrayutilities.materials.database.add_mass_from_NIST (db, nistfile)`

Read atoms standard mass and save it to the database.

`xrayutilities.materials.database.init_material_db (db)`

4.5.6 elements Module

4.5.7 lattice Module

module handling crystal lattice structures

class `xrayutilities.materials.lattice.Atom` (*name, num*)

Bases: object

f (*q, en='config'*)

function to calculate the atomic structure factor F

Parameter

qmomentum transfer

enenergy for which F should be calculated, if omitted the value from the xrayutilities configuration is used

Returns

f (float)

f0 (*q*)

f1 (*en*='config')

f2 (*en*='config')

xrayutilities.materials.lattice.**BCCLattice** (*aa*, *a*)

xrayutilities.materials.lattice.**BCTLattice** (*aa*, *a*, *c*)

xrayutilities.materials.lattice.**BaddeleyiteLattice** (*aa*, *ab*, *a*, *b*, *c*, *beta*,
deg=True)

xrayutilities.materials.lattice.**CuMnAsLattice** (*aa*, *ab*, *ac*, *a*, *b*, *c*)

xrayutilities.materials.lattice.**CubicFm3mBaF2** (*aa*, *ab*, *a*)

xrayutilities.materials.lattice.**CubicLattice** (*a*)

Returns a Lattice object representing a simple cubic lattice.

required input arguments:

alattice parameter

return value:an instance of Lattice class

xrayutilities.materials.lattice.**DiamondLattice** (*aa*, *a*)

xrayutilities.materials.lattice.**FCCLattice** (*aa*, *a*)

xrayutilities.materials.lattice.**GeneralPrimitiveLattice** (*a*, *b*, *c*, *alpha*, *beta*,
gamma)

xrayutilities.materials.lattice.**HCPLattice** (*aa*, *a*, *c*)

xrayutilities.materials.lattice.**Hexagonal3CLattice** (*aa*, *ab*, *a*, *c*)

xrayutilities.materials.lattice.**Hexagonal4HLattice** (*aa*, *ab*, *a*, *c*, *u*=0.1875,
v1=0.25, *v2*=0.4375)

xrayutilities.materials.lattice.**Hexagonal6HLattice** (*aa*, *ab*, *a*, *c*)

class xrayutilities.materials.lattice.**Lattice** (*a1*, *a2*, *a3*, *base=None*)

Bases: object

class Lattice: This object represents a Bravais lattice. A lattice consists of a base

ApplyStrain (*eps*)

Applies a certain strain on a lattice. The result is a change in the base vectors.

required input arguments:

epsa 3x3 matrix independent strain components

GetPoint (**args*)

determine lattice points with indices given in the argument

Examples

```
>>> xu.materials.Si.lattice.GetPoint(0,0,4)
array([ 0.      ,  0.      , 21.72416])
```

or

```
>>> xu.materials.Si.lattice.GetPoint((1,1,1))
array([ 5.43104,  5.43104,  5.43104])
```

ReciprocalLattice ()

UnitCellVolume ()

function to calculate the unit cell volume of a lattice (angstrom³)

class xrayutilities.materials.lattice.**LatticeBase** (*args, **keyargs)

Bases: list

The LatticeBase class implements a container for a set of points that form the base of a crystal lattice. An instance of this class can be treated as a simple container object.

append (atom, pos, occ=1.0, b=0.0)

add new Atom to the lattice base

Parameter

atom atom object to be added

pos position of the atom

occ occupancy (default=1.0)

bb-factor of the atom used as $\exp(-b*q^2/(4*\pi)^2)$ to reduce the intensity of this atom (only used in case of temp=0 in StructureFactor and chi calculation)

xrayutilities.materials.lattice.**NaumanniteLattice** (aa, ab, a, b, c)

xrayutilities.materials.lattice.**PerovskiteTypeRhombohedral** (aa, ab, ac, a, ang)

xrayutilities.materials.lattice.**QuartzLattice** (aa, ab, a, b, c)

xrayutilities.materials.lattice.**RockSaltLattice** (aa, ab, a)

xrayutilities.materials.lattice.**RockSalt_Cubic_Lattice** (aa, ab, a)

xrayutilities.materials.lattice.**RutileLattice** (aa, ab, a, c, u)

xrayutilities.materials.lattice.**TetragonalIndiumLattice** (aa, a, c)

xrayutilities.materials.lattice.**TetragonalTinLattice** (aa, a, c)

xrayutilities.materials.lattice.**TrigonalR3mh** (aa, a, c)

xrayutilities.materials.lattice.**WurtziteLattice** (aa, ab, a, c, u=0.375, biso=0.0)

xrayutilities.materials.lattice.**ZincBlendeLattice** (aa, ab, a)

4.5.8 material Module

class module implements a certain material

class xrayutilities.materials.material.**Alloy** (matA, matB, x)

Bases: xrayutilities.materials.material.Material

RelaxationTriangle (hkl, sub, exp)

function which returns the relaxation triangle for a Alloy of given composition. Reciprocal space coordinates are calculated using the user-supplied experimental class

Parameter

hkl Miller Indices

sub substrate material or lattice constant (Instance of Material class or float)

exp Experiment class from which the Transformation object and ndir are needed

Returns

qy,qz reciprocal space coordinates of the corners of the relaxation triangle

lattice_const_AB (latA, latB, x)

method to set the composition of the Alloy. x is the atomic fraction of the component B

x`xrayutilities.materials.material.Cij2Cijkl (cij)`

Converts the elastic constants matrix (tensor of rank 2) to the full rank 4 cijkl tensor.

required input arguments:`cij(6,6)` cij matrix as a numpy array**return value:**`cijkl(3,3,3,3)` cijkl tensor as numpy array`xrayutilities.materials.material.Cijkl2Cij (cijkl)`

Converts the full rank 4 tensor of the elastic constants to the (6,6) matrix of elastic constants.

required input arguments:`cijkl(3,3,3,3)` cijkl tensor as numpy array**return value:**`cij(6,6)` cij matrix as a numpy array**class** `xrayutilities.materials.material.CubicAlloy (matA, matB, x)`Bases: `xrayutilities.materials.material.Alloy`**ContentBsym** (*q_inp, q_perp, hkl, sur*)

function that determines the content of B in the alloy from the reciprocal space position of an asymmetric peak and also sets the content in the current material

Parameter

q_inp inplane peak position of reflection hkl of the alloy in reciprocal space**q_perp** perpendicular peak position of the reflection hkl of the alloy in reciprocal space**hkl** Miller indices of the measured asymmetric reflection**sur** Miller indices of the surface (determines the perpendicular direction)

Returns

content, **[a_inplane, a_perp, a_bulk_perp(x), eps_inplane, eps_perp]** : the content of B in the alloy determined from the input variables and the lattice constants calculated from the reciprocal space positions as well as the strain (eps) of the layer**ContentBsym** (*q_perp, hkl, inpr, asub, relax*)

function that determines the content of B in the alloy from the reciprocal space position of a symmetric peak. As an additional input the substrates lattice parameter and the degree of relaxation must be given

Parameter

q_perp perpendicular peak position of the reflection hkl of the alloy in reciprocal space**hkl** Miller indices of the measured symmetric reflection (also defines the surface normal)**inpr** Miller indices of a Bragg peak defining the inplane reference direction**asub** substrate lattice constant**relax** degree of relaxation (needed to obtain the content from symmetric reciprocal space position)

Returns

content the content of B in the alloy determined from the input variables

`xrayutilities.materials.material.CubicElasticTensor` (*c11, c12, c44*)

Assemble the 6x6 matrix of elastic constants for a cubic material from the three independent components of a cubic crystal

Parameter

c11,c12,c44 independent components of the elastic tensor of cubic materials

Returns

6x6 matrix with elastic constants

`xrayutilities.materials.material.GeneralUC` (*a=4, b=4, c=4, alpha=90, beta=90, gamma=90, name='General'*)

general material with primitive unit cell but possibility for different a,b,c and alpha,beta,gamma

Parameters

a,b,c unit cell extensions (Angstrom)

alpha angle between unit cell vectors b,c

beta angle between unit cell vectors a,c

gamma angle between unit cell vectors a,b

returns a Material object with the specified properties

`xrayutilities.materials.material.HexagonalElasticTensor` (*c11, c12, c13, c33, c44*)

Assemble the 6x6 matrix of elastic constants for a hexagonal material from the five independent components of a hexagonal crystal

Parameter

c11,c12,c13,c33,c44 independent components of the elastic tensor of a hexagonal material

Returns

6x6 matrix with elastic constants

class `xrayutilities.materials.material.Material` (*name, lat, cij=None, thetaDebye=None*)

Bases: object

ApplyStrain (*strain, **keyargs*)

B

GetMismatch (*mat*)

Calculate the mismatch strain between the material and a second material

Q (**hkl*)

Return the Q-space position for a certain material.

required input arguments:

hkl list or numpy array with the Miller indices (or Q(h,k,l) is also possible)

StructureFactor (*q, en='config', temp=0*)

calculates the structure factor of a material for a certain momentum transfer and energy at a certain temperature of the material

Parameter

q vectorial momentum transfer (vectors as list,tuple or numpy array are valid)

en energy in eV, if omitted the value from the xrayutilities configuration is used

temp temperature used for Debye-Waller-factor calculation

Returns

the complex structure factor

StructureFactorForEnergy (*q0, en, temp=0*)

calculates the structure factor of a material for a certain momentum transfer and a bunch of energies

Parameter

q0vectorial momentum transfer (vectors as list,tuple or numpy array are valid)

enlist, tuple or array of energy values in eV

temptemperature used for Debye-Waller-factor calculation

Returns

complex valued structure factor array

StructureFactorForQ (*q, en0='config', temp=0*)

calculates the structure factor of a material for a bunch of momentum transfers and a certain energy

Parameter

qvectorial momentum transfers; list of vectores (list, tuple or array) of length 3 e.g.:
(Si.Q(0,0,4),Si.Q(0,0,4.1),...) or numpy.array([Si.Q(0,0,4),Si.Q(0,0,4.1)])

en0energy value in eV, if omitted the value from the xrayutilities configuration is used

temptemperature used for Debye-Waller-factor calculation

Returns

complex valued structure factor array

a1

a2

a3

b1

b2

b3

beta (*en='config'*)

function to calculate the imaginary part of the deviation of the refractive index from 1 ($n=1-\delta+i\beta$)

Parameter

enx-ray energy eV, if omitted the value from the xrayutilities configuration is used

Returns

beta (float)

chi0 (*en='config'*)

calculates the complex χ_0 values often needed in simulations. They are closely related to δ and β ($n = 1 + \chi_0/2 + i\chi''_0/2$ vs. $n = 1 - \delta + i\beta$)

chih (*q, en='config', temp=0, polarization='S'*)

calculates the complex polarizability of a material for a certain momentum transfer and energy

Parameter

qmomentum transfer in (1/Å)

enx-ray energy in eV, if omitted the value from the xrayutilities configuration is used

temptemperature used for Debye-Waller-factor calculation

polarizationeither 'S' (default) sigma or 'P' pi polarization

Returns

(abs(chih_real),abs(chih_imag)) complex polarizability

critical_angle (*en*='config', *deg*=True)

calculate critical angle for total external reflection

Parameter

enenergy of the x-rays, if omitted the value from the xrayutilities configuration is used

degreturn angle in degree if True otherwise radians (default:True)

Returns

Angle of total external reflection

dTheta (*Q*, *en*='config')

function to calculate the refractive peak shift

Parameter

Qmomentum transfer (1/Å)

enx-ray energy (eV), if omitted the value from the xrayutilities configuration is used

Returns

deltaThetapeak shift in degree

delta (*en*='config')

function to calculate the real part of the deviation of the refractive index from 1 ($n=1-\delta+i\beta$)

Parameter

enx-ray energy eV, if omitted the value from the xrayutilities configuration is used

Returns

delta (float)

idx_refraction (*en*='config')

function to calculate the complex index of refraction of a material in the x-ray range

Parameter

enenergy of the x-rays, if omitted the value from the xrayutilities configuration is used

Returns

n (complex)

lam

mu

nu

`xrayutilities.materials.material.PseudomorphicMaterial` (*submat*, *layermat*)

This function returns a material whos lattice is pseudomorphic on a particular substrate material. This function works meanwhile only for cubic materials.

required input arguments:

submatsubstrate material

layermatbulk material of the layer

return value:An instance of Material holding the new pseudomorphically strained material.

`xrayutilities.materials.material.index_map_ij2ijk1` (*ij*)

`xrayutilities.materials.material.index_map_ijk12ij` (*i*, *j*)

4.5.9 predefined_materials Module

class xrayutilities.materials.predefined_materials.**SiGe**(*x*)
 Bases: xrayutilities.materials.material.CubicAlloy
lattice_const_AB(*latA, latB, x*)
 method to calculate the lattice parameter of the SiGe alloy with composition $\text{Si}_{1-x}\text{Ge}_x$
x

4.6 math Package

4.6.1 math Package

4.6.2 fit Module

module with a function wrapper to `scipy.optimize.leastsq` for fitting of a 2D function to a peak or a 1D Gauss fit with the odr package

`xrayutilities.math.fit.fit_peak2d(x, y, data, start, drange, fit_function, maxfev=2000)`
 fit a two dimensional function to a two dimensional data set e.g. a reciprocal space map

Parameters

x,ydata coordinates (do NOT need to be regularly spaced)
datadata set used for fitting (e.g. intensity at the data coords)
startset of starting parameters for the fit used as first parameter of function `fit_function`
drangelimits for the data ranges used in the fitting algorithm e.g. it is clever to use only a small region around the peak which should be fitted: `[xmin,xmax,ymin,ymax]`
fit_functionfunction which should be fitted must accept the parameters `(x,y,*params)`

Returns

(fitparam,cov)the set of fitted parameters and covariance matrix

`xrayutilities.math.fit.gauss_fit(xdata, ydata, iparams=[], maxit=200)`
 Gauss fit function using odr-pack wrapper in scipy similar to :https://github.com/tiagopereira/python_tips/wiki/Scipy%3A-curve-fitting

Parameters

xdataxcoordinates of the data to be fitted
ydataycoordinates of the data which should be fit

keyword parameters:

iparamsinitial paramters for the fit (determined automatically if nothing is given)
maxitmaximal iteration number of the fit

Returns

`params,sd_params,itlim`

the Gauss parameters as defined in function `Gauss1d(x, *param)` and their errors of the fit, as well as a boolean flag which is false in the case of a successful fit

4.6.3 functions Module

module with several common function needed in xray data analysis

`xrayutilities.math.functions.Debye1(x)`

function to calculate the first Debye function as needed for the calculation of the thermal Debye-Waller-factor by numerical integration

for definition see: http://en.wikipedia.org/wiki/Debye_function

$$D1(x) = (1/x) \int_0^x t / (\exp(t)-1) dt$$

Parameters

x argument of the Debye function (float)

Returns

D1(x) float value of the Debye function

`xrayutilities.math.functions.Gauss1d(x, *p)`

function to calculate a general one dimensional Gaussian

Parameters

p list of parameters of the Gaussian [XCEN,SIGMA,AMP,BACKGROUND] for information: $SIGMA = FWHM / (2 * \sqrt{2 * \log(2)})$

x coordinate(s) where the function should be evaluated

Returns

the value of the Gaussian described by the parameters p at position x

`xrayutilities.math.functions.Gauss1d_der_p(x, *p)`

function to calculate the derivative of a Gaussian with respect the parameters p

for parameter description see Gauss1d

`xrayutilities.math.functions.Gauss1d_der_x(x, *p)`

function to calculate the derivative of a Gaussian with respect to x

for parameter description see Gauss1d

`xrayutilities.math.functions.Gauss2d(x, y, *p)`

function to calculate a general two dimensional Gaussian

Parameters

p list of parameters of the Gauss-function [XCEN,YCEN,SIGMAX,SIGMAY,AMP,BACKGROUND,ANGLE] $SIGMA = FWHM / (2 * \sqrt{2 * \log(2)})$ ANGLE = rotation of the X,Y direction of the Gaussian in radians

x,y coordinate(s) where the function should be evaluated

Returns

the value of the Gaussian described by the parameters p at position (x,y)

`xrayutilities.math.functions.Lorentz1d(x, *p)`

function to calculate a general one dimensional Lorentzian

Parameters

p list of parameters of the Lorentz-function [XCEN,FWHM,AMP,BACKGROUND]

x,y coordinate(s) where the function should be evaluated

Returns

the value of the Lorentian described by the parameters p at position (x,y)

`xrayutilities.math.functions.Lorentz2d(x, y, *p)`

function to calculate a general two dimensional Lorentzian

Parameters

plist of parameters of the Lorentz-function [XCEN,YCEN,FWHMX,FWHMY,AMP,BACKGROUND,ANGLE]

ANGLE = rotation of the X,Y direction of the Lorentzian in radians

x,ycoordinate(s) where the function should be evaluated

Returns

the value of the Lorentian described by the parameters p at position (x,y)

`xrayutilities.math.functions.TwoGauss2d(x, y, *p)`

function to calculate two general two dimensional Gaussians

Parameters

plist of parameters of the Gauss-function [XCEN1,YCEN1,SIGMAX1,SIGMAY1,AMP1,ANGLE1,XCEN2,YCEN2]

SIGMA = FWHM / (2*sqrt(2*log(2))) ANGLE = rotation of the X,Y direction of

the Gaussian in radians

x,ycoordinate(s) where the function should be evaluated

Return

the value of the Gaussian described by the parameters p at position (x,y)

`xrayutilities.math.functions.kill_spike(data, threshold=2.0)`

function to smooth ****single**** data points which differ from the average of the neighboring data points by more than the threshold factor. Such spikes will be replaced by the mean value of the next neighbors.

Warning: Use this function carefully not to manipulate your data!

Parameters

data1d numpy array with experimental data

thresholdthreshold factor to identify strange data points

Returns

1d data-array with spikes removed

`xrayutilities.math.functions.smooth(x, n)`

function to smooth an array of data by averaging N adjacent data points

Parameters

x1D data array

nnumber of data points to average

Returns

xsmoothsmoothed array with same length as x

4.6.4 transforms Module

class `xrayutilities.math.transforms.AxisToZ(newzaxis)`

Bases: `xrayutilities.math.transforms.CoordinateTransform`

Creates a coordinate transformation to move a certain axis to the z-axis. The rotation is done along the great circle. The x-axis of the new coordinate frame is created to be normal to the new and original z-axis. The new y-axis is create in order to obtain a right handed coordinate system.

`xrayutilities.math.transforms.Cij2Cijkl(cij)`

Converts the elastic constants matrix (tensor of rank 2) to the full rank 4 cijkl tensor.

required input arguments:

cij(6,6) cij matrix as a numpy array

return value:

cijkl(3,3,3,3) cijkl tensor as numpy array

`xrayutilities.math.transforms.Cijkl2Cij` (*cijkl*)

Converts the full rank 4 tensor of the elastic constants to the (6,6) matrix of elastic constants.

required input arguments:

cijkl(3,3,3,3) cijkl tensor as numpy array

return value:

cij(6,6) cij matrix as a numpy array

class `xrayutilities.math.transforms.CoordinateTransform` (*v1*, *v2*, *v3*)

Bases: `xrayutilities.math.transforms.Transform`

Create a Transformation object which transforms a point into a new coordinate frame. The new frame is determined by the three vectors *v1*/norm(*v1*), *v2*/norm(*v2*) and *v3*/norm(*v3*), which need to be orthogonal!

class `xrayutilities.math.transforms.Transform` (*matrix*)

Bases: `object`

inverse (**args*)

performs inverse transformation a vector, matrix or tensor of rank 4

Parameters

***args: object to transform, list or numpy array of shape(n,) (n,n), (n,n,n,n) where n is the rank of the transformation matrix**

`xrayutilities.math.transforms.XRotation` (*alpha*, *deg=True*)

Returns a transform that represents a rotation about the x-axis by an angle *alpha*. If *deg=True* the angle is assumed to be in degree, otherwise the function expects radians.

`xrayutilities.math.transforms.YRotation` (*alpha*, *deg=True*)

Returns a transform that represents a rotation about the y-axis by an angle *alpha*. If *deg=True* the angle is assumed to be in degree, otherwise the function expects radians.

`xrayutilities.math.transforms.ZRotation` (*alpha*, *deg=True*)

Returns a transform that represents a rotation about the z-axis by an angle *alpha*. If *deg=True* the angle is assumed to be in degree, otherwise the function expects radians.

`xrayutilities.math.transforms.index_map_ij2ijkl` (*ij*)

`xrayutilities.math.transforms.index_map_ijkl2ij` (*i*, *j*)

`xrayutilities.math.transforms.mycross` (*vec*, *mat*)

function implements the cross-product of a vector with each column of a matrix

`xrayutilities.math.transforms.rotarb` (*vec*, *axis*, *ang*, *deg=True*)

function implements the rotation around an arbitrary axis by an angle *ang* positive rotation is anti-clockwise when looking from positive end of axis vector

Parameter

vec numpy.array or list of length 3

axis numpy.array or list of length 3

ang rotation angle in degree (*deg=True*) or in rad (*deg=False*)

deg boolean which determines the input format of *ang* (default: *True*)

Returns

rotvec rotated vector as numpy.array

Example

```
>>> rotarb([1,0,0],[0,0,1],90)
array([ 6.12323400e-17,  1.00000000e+00,  0.00000000e+00])
```

`xrayutilities.math.transforms.tensorprod(vec1, vec2)`
function implements an elementwise multiplication of two vectors

4.6.5 vector Module

module with vector operations, mostly numpy functionality is used for the vector operation itself, however custom error checking is done to ensure vectors of length 3.

`xrayutilities.math.vector.VecAngle(v1, v2, deg=False)`
calculate the angle between two vectors. The following formula is used $v1.v2 = \text{norm}(v1)*\text{norm}(v2)*\cos(\alpha)$

$\alpha = \arccos((v1.v2)/(\text{norm}(v1)*\text{norm}(v2)))$

required input arguments:

v1 vector as numpy array or list

v2 vector as numpy array or list

optional keyword arguments:

deg(default: false) return result in degree otherwise in radians

return value: float value with the angle inclined by the two vectors

`xrayutilities.math.vector.VecDot(v1, v2)`
Calculate the vector dot product.

required input arguments:

v1 vector as numpy array or list

v2 vector as numpy array or list

return value: float value

`xrayutilities.math.vector.VecNorm(v)`
Calculate the norm of a vector.

required input arguments:

v vector as list or numpy array

return value: float holding the vector norm

`xrayutilities.math.vector.VecUnit(v)`
Calculate the unit vector of v.

required input arguments:

v vector as list or numpy array

return value: numpy array with the unit vector

`xrayutilities.math.vector.getSyntax(vec)`
returns vector direction in the syntax 'x+' 'z-' or equivalents therefore works only for principle vectors of the coordinate system like e.g. [1,0,0] or [0,2,0]

Parameters

string[xyz][+-]

Returns

vector along the given direction as numpy array

`xrayutilities.math.vector.getVector (string)`

returns unit vector along a rotation axis given in the syntax 'x+' 'z-' or equivalents

Parameters

string[xyz][+-]

Returns

vector along the given direction as numpy array

4.7 xrayutilities

4.7.1 xrayutilities Package

xrayutilities Package

xrayutilities is a Python package for assisting with x-ray diffraction experiments. Its the python package included in *xrayutilities*.

It helps with planning experiments as well as analyzing the data.

Authors Dominik Kriegner <dominik.kriegner@gmail.com> and Eugen Wintersberger <eugen.wintersberger@desy.de>

config Module

module to parse xrayutilities user-specific config file the parsed values are provide as global constants for the use in other parts of xrayutilities. The config file with the default constants is found in the python installation path of xrayutilities. It is however not recommended to change things there, instead the user-specific config file ~/.xrayutilities.conf or the local xrayutilities.conf file should be used.

exception Module

xrayutilities derives its own exceptions which are raised upon wrong input when calling one of xrayutilities functions. none of the pre-defined exceptions is made for that purpose.

exception `xrayutilities.exception.InputError (msg)`

Bases: `exceptions.Exception`

Exception raised for errors in the input. Either wrong datatype not handled by `TypeError` or missing mandatory keyword argument (Note that the obligation to give keyword arguments might depend on the value of the arguments itself)

Attributes `expr` – input expression in which the error occurred :`msg`: – explanation of the error

experiment Module

module helping with planning and analyzing experiments

various classes are provided for

* describing experiments * calculating angular coordinates of Bragg reflections * converting angular coordinates to Q-space and vice versa * simulating powder diffraction patterns for materials

class `xrayutilities.experiment.Experiment (ipdir, ndir, **keyargs)`

Bases: `object`

base class for describing experiments users should use the derived classes: `HXRD`, `GID`, `Powder`

Ang2HKL (**args, **kwargs*)

angular to (h,k,l) space conversion. It will set the UB argument to Ang2Q and pass all other parameters unchanged. See Ang2Q for description of the rest of the arguments.

Parameters

****kwargs: optional keyword arguments**

Breciprocal space conversion matrix of a Material. you can specify the matrix B (default identity matrix) shape needs to be (3,3)

matMaterial object to use to obtain a B matrix (e.g. xu.materials.Si) can be used as alternative to the B keyword argument B is favored in case both are given

Uorientation matrix U can be given if none is given the orientation defined in the Experiment class is used.

dettypedetector type: one of ('point', 'linear', 'area') decides which routine of Ang2Q to call default 'point'

Returns

H K L coordinates as numpy.ndarray with shape (*, 3) where * corresponds to the number of points given in the input (*args)

Q2Ang (*qvec*)

TiltAngle (*q, deg=True*)

TiltAngle(q,deg=True): Return the angle between a q-space position and the surface normal.

Parameters

qlist or numpy array with the reciprocal space position

optional keyword arguments:

degTrue/False whether the return value should be in degree or radians :(default: True)

Transform (*v*)

transforms a vector, matrix or tensor of rank 4 (e.g. elasticity tensor) to the coordinate frame of the Experiment class.

Parameters

vobject to transform, list or numpy array of shape (n,) (n,n), (n,n,n,n) where n is the rank of the transformation matrix

Returns

transformed object of the same shape as v

energy

wavelength

class xrayutilities.experiment.GID (*idir, ndir, **keyargs*)

Bases: xrayutilities.experiment.Experiment

class describing grazing incidence x-ray diffraction experiments the class helps with calculating the angles of Bragg reflections as well as it helps with analyzing measured data

the class describes a four circle (alpha_i,azimuth,twotheta,beta) goniometer to help with GID experiments at the ROTATING ANODE. 3D data can be treated with the use of linear and area detectors. see help self.Ang2Q

Ang2Q (*ai, phi, tt, beta, **kwargs*)

angular to momentum space conversion for a point detector. Also see help GID.Ang2Q for procedures which treat line and area detectors

Parameters

ai,phi,tt,beta sample and detector angles as numpy array, lists or Scalars must be given. all arguments must have the same shape or length

****kwargs: optional keyword arguments**

delta giving delta angles to correct the given ones for misalignment delta must be an numpy array or list of length 4. used angles are than ai,phi,tt,beta - delta

UB matrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: identity matrix)

wl x-ray wavelength in angstroem (default: self._wl)

degflag to tell if angles are passed as degree (default: True)

Returns

reciprocal space positions as numpy.ndarray with shape (* , 3) where * corresponds to the number of points given in the input

Q2Ang (*Q, trans=True, deg=True, **kwargs*)

calculate the GID angles needed in the experiment the inplane reference direction defines the direction were the reference direction is parallel to the primary beam (i.e. lattice planes perpendicular to the beam)

Parameters

Q a list or numpy array of shape (3) with q-space vector components

optional keyword arguments:

trans True/False apply coordinate transformation on Q

deg True/False (default True) determines if the angles are returned in radians or degrees

Returns

a numpy array of shape (4) with the four GID scattering angles which are [alpha_i, azimuth, twotheta, beta]

alpha_i incidence angle to surface (at the moment always 0)

azimuth sample rotation with respect to the inplane reference direction

twotheta scattering angle

beta exit angle from surface (at the moment always 0)

class xrayutilities.experiment.GID_ID10B (*idir, ndir, **keyargs*)

Bases: xrayutilities.experiment.GID

class describing grazing incidence x-ray diffraction experiments the class helps with calculating the angles of Bragg reflections as well as it helps with analyzing measured data

the class describes a four circle (theta, omega, delta, gamma) goniometer to help with GID experiments at ID10B / ESRF. 3D data can be treated with the use of linear and area detectors. see help self.Ang2Q

Ang2Q (*th, om, delta, gamma, **kwargs*)

angular to momentum space conversion for a point detector. Also see help GID_ID10B.Ang2Q for procedures which treat line and area detectors

Parameters

th, om, delta, gamma sample and detector angles as numpy array, lists or Scalars must be given. all arguments must have the same shape or length

****kwargs: optional keyword arguments**

delta giving delta angles to correct the given ones for misalignment delta must be an numpy array or list of length 4. used angles are than th,om,delta,gamma - delta

UBmatrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: identity matrix)

wlx-ray wavelength in angstroem (default: self._wl)

degflag to tell if angles are passed as degree (default: True)

Returns

reciprocal space positions as numpy.ndarray with shape (*, 3) where * corresponds to the number of points given in the input

Q2Ang (*Q*, *trans=True*, *deg=True*, ***kwargs*)

calculate the GID angles needed in the experiment the inplane reference direction defines the direction were the reference direction is parallel to the primary beam (i.e. lattice planes perpendicular to the beam)

Parameters

Qa list or numpy array of shape (3) with q-space vector components

optional keyword arguments:

transTrue/False apply coordinate transformation on Q

degTrue/Flase (default True) determines if the angles are returned in radians or degrees

Returns

a numpy array of shape (4) with the four GID scattering angles which are (theta,omega,delta,gamma)

thetaincidence angle to surface (at the moment always 0)

omegasample rotation with respect to the inplane reference direction

deltaexit angle from surface (at the moment always 0)

gammascattering angle

class xrayutilities.experiment.**GISAXS** (*idir*, *ndir*, ***keyargs*)

Bases: xrayutilities.experiment.Experiment

class describing grazing incidence x-ray diffraction experiments the class helps with calculating the angles of Bragg reflections as well as it helps with analyzing measured data

the class describes a three circle (alpha_i,twotheta,beta) goniometer to help with GISAXS experiments at the ROTATING ANODE. 3D data can be treated with the use of linear and area detectors. see help self.Ang2Q

Ang2Q (*ai*, *tt*, *beta*, ***kwargs*)

angular to momentum space conversion for a point detector. Also see help GISAXS.Ang2Q for procedures which treat line and area detectors

Parameters

ai,tt,betasample and detector angles as numpy array, lists or Scalars must be given.

all arguments must have the same shape or length

****kwargs: optional keyword arguments**

deltagiving delta angles to correct the given ones for misalignment delta must be an numpy array or list of length 3. used angles are than ai,tt,beta - delta

UBmatrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: identity matrix)

wlx-ray wavelength in angstroem (default: self._wl)

degflag to tell if angles are passed as degree (default: True)

Returns

reciprocal space positions as `numpy.ndarray` with shape `(*, 3)` where `*` corresponds to the number of points given in the input

Q2Ang (*Q*, *trans=True*, *deg=True*, ***kwargs*)

class `xrayutilities.experiment.HXRD` (*idir*, *ndir*, *geometry='hi_lo'*, ***keyargs*)

Bases: `xrayutilities.experiment.Experiment`

class describing high angle x-ray diffraction experiments the class helps with calculating the angles of Bragg reflections as well as helps with analyzing measured data

the class describes a two circle (omega,twotheta) goniometer to help with coplanar x-ray diffraction experiments. Nevertheless 3D data can be treated with the use of linear and area detectors. see help `self.Ang2Q`

Ang2Q (*om*, *tt*, ***kwargs*)

angular to momentum space conversion for a point detector. Also see help `HXRD.Ang2Q` for procedures which treat line and area detectors

Parameters

om,tt sample and detector angles as numpy array, lists or Scalars must be given. all arguments must have the same shape or length

****kwargs: optional keyword arguments**

delta giving delta angles to correct the given ones for misalignment delta must be an numpy array or list of length 2. used angles are than `om,tt - delta`

UB matrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: identity matrix)

wl x-ray wavelength in angstroem (default: `self._wl`)

degflag to tell if angles are passed as degree (default: True)

Returns

reciprocal space positions as `numpy.ndarray` with shape `(*, 3)` where `*` corresponds to the number of points given in the input

Q2Ang (**Q*, ***keyargs*)

Convert a reciprocal space vector Q to COPLANAR scattering angles. The keyword argument `trans` determines whether Q should be transformed to the experimental coordinate frame or not.

Parameters

Q a list, tuple or numpy array of shape (3) with q-space vector components or 3 separate lists with `qx,qy,qz`

optional keyword arguments:

trans True/False apply coordinate transformation on Q (default True)

deg True/False (default True) determines if the angles are returned in radians or degrees

geometry determines the scattering geometry:

- “hi_lo” high incidence and low exit

- “lo_hi” low incidence and high exit

- “real” general geometry with angles determined by q-coordinates (azimuth); this and upper geomet

–“realTilt” general geometry with angles determined by q-coordinates (tilt); returns [omega,chi,phi,twotheta]

defaultself.geometry

refracboolean to determine if refraction is taken into account :default: False if True then also a material must be given

matMaterial object; needed to obtain its optical properties for refraction correction, otherwise not used

full_outputboolean to determine if additional output is given to determine scattering angles more accurately in case refraction is set to True :default: False

fi,fdif refraction correction is applied one can optionally specify the facet through which the beam enters (fi) and exits (fd) fi, fd must be the surface normal vectors (not transformed & not necessarily normalized). If omitted the normal direction of the experiment is used.

Returns

a numpy array of shape (4) with four scattering angles which are [omega,chi,phi,twotheta]

omegaincidence angle with respect to surface

chisample tilt for the case of non-coplanar geometry

phisample azimuth with respect to inplane reference direction

twothetascattering angle/detector angle

if full_output: a numpy array of shape (6) with five angles which are [omega,chi,phi,twotheta,psi_i,psi_d]

psi_ioffset of the incidence beam from the scattering plane due to refraction

psi_doffset of the diffracted beam from the scattering plane due to refraction

class xrayutilities.experiment.**NonCOP** (*idir, ndir, **keyargs*)

Bases: xrayutilities.experiment.Experiment

class describing high angle x-ray diffraction experiments the class helps with calculating the angles of Bragg reflections as well as helps with analyzing measured data for NON-COPLANAR measurements, where the tilt is used to align asymmetric peaks, like in the case of a polefigure measurement.

the class describes a four circle (omega,twotheta) goniometer to help with x-ray diffraction experiments. Linear and area detectors can be treated as described in “help self.Ang2Q”

Ang2Q (*om, chi, phi, tt, **kwargs*)

angular to momentum space conversion for a point detector. Also see help NonCOP.Ang2Q for procedures which treat line and area detectors

Parameters

om,chi,phi,ttsample and detector angles as numpy array, lists or Scalars must be given. all arguments must have the same shape or length

****kwargs: optional keyword arguments**

deltagiving delta angles to correct the given ones for misalignment delta must be a numpy array or list of length 4. used angles are than om,chi,phi,tt - delta

UBmatrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: identity matrix)

wlx-ray wavelength in angstroem (default: self._wl)

degflag to tell if angles are passed as degree (default: True)

Returns

reciprocal space positions as `numpy.ndarray` with shape `(*, 3)` where `*` corresponds to the number of points given in the input

Q2Ang (**Q, **keyargs*)

Convert a reciprocal space vector `Q` to NON-COPLANAR scattering angles. The keyword argument `trans` determines whether `Q` should be transformed to the experimental coordinate frame or not.

Parameters

Q a list, tuple or `numpy` array of shape `(3)` with q-space vector components or 3 separate lists with `qx, qy, qz`

optional keyword arguments:

trans True/False apply coordinate transformation on `Q` (default True)

deg True/False (default True) determines if the angles are returned in radians or degree

Returns

a `numpy` array of shape `(4)` with four scattering angles which are `[omega, chi, phi, twotheta]`

omega sample rocking angle

chi sample tilt

phi sample azimuth

twotheta scattering angle (detector)

class `xrayutilities.experiment.Powder` (*mat, **keyargs*)

Bases: `xrayutilities.experiment.Experiment`

Experimental class for powder diffraction This class is able to simulate a powder spectrum for the given material

Convolute (*stepwidth, width, min=0, max=None*)

Convolute the intensity positions with Gaussians with width in momentum space of “width”. returns array of angular positions with corresponding intensity

theta array with angular positions

int intensity at the positions `ttheta`

PowderIntensity (*tt_cutoff=180*)

Calculates the powder intensity and positions up to an angle of `tt_cutoff` (deg) and stores the result in:

data array with intensities

ang angular position of intensities

qpos reciprocal space position of intensities

Q2Ang (*qpos, deg=True*)

Converts reciprocal space values to theta angles

class `xrayutilities.experiment.QConversion` (*sampleAxis, detectorAxis, r_i, **kwargs*)

Bases: `object`

Class for the conversion of angular coordinates to momentum space for arbitrary goniometer geometries

the class is configured with the initialization and does provide three distinct routines for conversion to momentum space for

* point detector: `point(...)` or `__call__()` * linear detector: `linear(...)` * area detector: `area(...)`

`linear()` and `area()` can only be used after the `init_linear()` or `init_area()` routines were called

UB

area (*args, **kwargs)

angular to momentum space conversion for a area detector the center pixel defined by the init_area routine must be in direction of self.r_i when detector angles are zero

the detector geometry must be initialized by the init_area(...) routine

Parameters

***args:** sample and detector angles as numpy array, lists or Scalars

in total len(self.sampleAxis)+len(detectorAxis) must be given always starting with the outer most circle all arguments must have the same shape or length

sAnglessample circle angles, number of arguments must correspond to len(self.sampleAxis)

dAnglesdetector circle angles, number of arguments must correspond to len(self.detectorAxis)

****kwargs:** possible keyword arguments

deltagiving delta angles to correct the given ones for misalignment delta must be an numpy array or list of len(*args) used angles are than *args - delta

UBmatrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: self.UB)

roiregion of interest for the detector pixels; e.g. [100,900,200,800] :(default: self._area_roi)

Navnumber of channels to average to reduce data size e.g. [2,2] :(default: self._area_nav)

wlx-ray wavelength in angstroem (default: self._wl)

degflag to tell if angles are passed as degree (default: True)

Returns

reciprocal space position of all detector pixels in a numpy.ndarray of shape ((self._area_roi[1]-self._area_roi[0]+1)*(self._area_roi[3]-self._area_roi[2]+1) , 3) where detectorDir1 is the fastest varying

detectorAxis

property handler for _detectorAxis

Returns

list of detector axis following the syntax /[xyz][+]/

energy

init_area (detectorDir1, detectorDir2, cch1, cch2, Nch1, Nch2, distance=None, pwidth1=None, pwidth2=None, chpdeg1=None, chpdeg2=None, detrot=0, tiltazimuth=0, tilt=0, **kwargs)

initialization routine for area detectors detector direction as well as distance and pixel size or channels per degree must be given. Two separate pixel sizes and channels per degree for the two orthogonal directions can be given

Parameters

detectorDir1direction of the detector (along the pixel direction 1); e.g. 'z+' means higher pixel numbers at larger z positions

detectorDir2direction of the detector (along the pixel direction 2); e.g. 'x+'

cch1,2center pixel, in direction of self.r_i at zero detectorAngles

Nch1number of detector pixels along direction 1

Nch2number of detector pixels along direction 2

distance distance of center pixel from center of rotation

pwidth1,2 width of one pixel (same unit as distance)

chpdeg1,2 channels per degree (only absolute value is relevant) sign determined through detectorDir1,2

detrot angle of the detector rotation around primary beam direction (used to correct misalignments)

tiltazimuth direction of the tilt vector in the detector plane (in degree)

tilt tilt of the detector plane around an axis normal to the direction given by the tiltazimuth

Note: Note: Either distance and pwidth1,2 or chpdeg1,2 must be given !!

Note: Note: the channel numbers run from 0 .. NchX-1

****kwargs: optional keyword arguments**

Nav number of channels to average to reduce data size (default: [1,1])

roi region of interest for the detector pixels; e.g. [100,900,200,800]

init_linear (*detectorDir*, *cch*, *Nchannel*, *distance=None*, *pixelwidth=None*, *chpdeg=None*, *tilt=0*, ***kwargs*)

initialization routine for linear detectors detector direction as well as distance and pixel size or channels per degree must be given.

Parameters

detectorDir direction of the detector (along the pixel array); e.g. 'z+'

cch center channel, in direction of self.r_i at zero detectorAngles

Nchannel total number of detector channels

distance distance of center channel from center of rotation

pixelwidth width of one pixel (same unit as distance)

chpdeg channels per degree (only absolute value is relevant) sign determined through detectorDir

!! Either distance and pixelwidth or chpdeg must be given !!

tilt tilt of the detector axis from the detectorDir (in degree)

Note: Note: the channel numbers run from 0 .. Nchannel-1

****kwargs: optional keyword arguments**

Nav number of channels to average to reduce data size (default: 1)

roi region of interest for the detector pixels; e.g. [100,900]

linear (**args*, ***kwargs*)

angular to momentum space conversion for a linear detector the cch of the detector must be in direction of self.r_i when detector angles are zero

the detector geometry must be initialized by the init_linear(...) routine

Parameters

***args: sample and detector angles as numpy array, lists or Scalars**

in total `len(self.sampleAxis)+len(detectorAxis)` must be given always starting with the outer most circle all arguments must have the same shape or length

sAnglessample circle angles, number of arguments must correspond to `len(self.sampleAxis)`

dAnglesdetector circle angles, number of arguments must correspond to `len(self.detectorAxis)`

****kwargs: possible keyword arguments**

deltagiving delta angles to correct the given ones for misalignment delta must be an numpy array or list of `len(*args)` used angles are than `*args - delta`

UBmatrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: self.UB)

Navnumber of channels to average to reduce data size (default: self._linear_nav)

roiregion of interest for the detector pixels; e.g. [100,900] (default: self._linear_roi)

wlx-ray wavelength in angstroem (default: self._wl)

degflag to tell if angles are passed as degree (default: True)

Returns

reciprocal space position of all detector pixels in a numpy.ndarray of shape `((*)(self._linear_roi[1]-self._linear_roi[0]+1), 3)`

point (**args*, ***kwargs*)

angular to momentum space conversion for a point detector located in direction of self.r_i when detector angles are zero

Parameters

***args: sample and detector angles as numpy array, lists**

or Scalars in total `len(self.sampleAxis)+len(detectorAxis)` must be given, always starting with the outer most circle. all arguments must have the same shape or length

sAnglessample circle angles, number of arguments must correspond to `len(self.sampleAxis)`

dAnglesdetector circle angles, number of arguments must correspond to `len(self.detectorAxis)`

****kwargs: optional keyword arguments**

deltagiving delta angles to correct the given ones for misalignment delta must be an numpy array or list of `len(*args)` used angles are than `*args - delta`

UBmatrix for conversion from (hkl) coordinates to Q of sample used to determine not Q but (hkl) :(default: self.UB)

wlx-ray wavelength in angstroem (default: self._wl)

degflag to tell if angles are passed as degree :(default: True)

Returns

reciprocal space positions as numpy.ndarray with shape `(*, 3)` where * corresponds to the number of points given in the input

sampleAxis

property handler for `_sampleAxis`

Returns

list of sample axis following the syntax `/[xyzk][+-]/`

wavelength

gridder Module

class `xrayutilities.gridder.Gridder`

Bases: `object`

KeepData (*bool*)

Normalize (*bool*)

class `xrayutilities.gridder.Gridder1D` (*nx*)

Bases: `xrayutilities.gridder.Gridder`

Clear ()

data

xaxis

Returns the xaxis of the gridder the returned values correspond to the center of the data bins used by the `numpy.histogram` function

`xrayutilities.gridder.axis` (*min_value*, *max_value*, *n*)

Compute the a grid axis.

Parameters

Min_value axis minimum value

Max_value axis maximum value

N number of steps

`xrayutilities.gridder.check_array` (*a*, *dtype*)

Check if an array fits the requirements for the C-code and returns it back to the callee. Such arrays must be aligned and C_CONTIGUOUS which means that they have to follow C-ordering.

Parameters

A array to check

Dtype numpy data type

`xrayutilities.gridder.delta` (*min_value*, *max_value*, *n*)

Compute the stepsize along an axis of a grid.

Parameters

Min_value axis minimum value

Max_value axis maximum value

N number of steps

`xrayutilities.gridder.ones` (**args*)

Compute ones for matrix generation. The shape is determined by the number of input arguments.

gridder2d Module

class `xrayutilities.gridder2d.Gridder2D` (*nx*, *ny*)

Bases: `xrayutilities.gridder.Gridder`

Clear()

SetResolution (*nx, ny*)

Reset the resolution of the gridder. In this case the original data stored in the object will be deleted.

Parameters

Nx number of points in x-direction

Ny number of points in y-direction

data

xaxis

xmatrix

yaxis

ymatrix

gridder3d Module

class xrayutilities.gridder3d.**Gridder3D** (*nx, ny, nz*)

Bases: xrayutilities.gridder.Gridder

SetResolution (*nx, ny, nz*)

xaxis

xmatrix

yaxis

ymatrix

zaxis

zmatrix

normalize Module

module to provide functions that perform block averaging of intensity arrays to reduce the amount of data (mainly for PSD and CCD measurements

and

provide functions for normalizing intensities for

* count time * absorber (user-defined function) * monitor * flatfield correction

class xrayutilities.normalize.**IntensityNormalizer** (*det, **keyargs*)

Bases: object

generic class for correction of intensity (point detector, or MCA, single CCD frames) for count time and absorber factors the class must be supplied with a absorber correction function and works with data structures provided by xrayutilities.io classes or the corresponding objects from hdf5 files read by pytables

absfun

absfun property handler returns the costum correction function or None

avmon

av_mon property handler returns the value of the average monitor or None if average is calculated from the monitor field

darkfield

flatfield property handler returns the current set darkfield of the detector or None if not set

det

det property handler returns the detector field name

flatfield

flatfield property handler returns the current set flatfield of the detector or None if not set

mon

mon property handler returns the monitor field name or None if not set

time

time property handler returns the count time or the field name of the count time or None if time is not set

`xrayutilities.normalize.blockAverage1D` (*data*, *Nav*)

perform block average for 1D array/list of Scalar values all data are used. at the end of the array a smaller cell may be used by the averaging algorithm

Parameter

datadata which should be contracted (length N)

Navnumber of values which should be averaged

Returns

block averaged numpy array of data type numpy.double (length ceil(N/Nav))

`xrayutilities.normalize.blockAverage2D` (*data2d*, *Nav1*, *Nav2*, ****kwargs**)

perform a block average for 2D array of Scalar values all data are used therefore the margin cells may differ in size

Parameter

data2darray of 2D data shape (N,M)

Nav1,Nav2a field of (Nav1 x Nav2) values is contracted

****kwargs: optional keyword argument**

roiregion of interest for the 2D array. e.g. [20,980,40,960] N = 980-20; M = 960-40

Returns

block averaged numpy array with type numpy.double with shape (ceil(N/Nav1), ceil(M/Nav2))

`xrayutilities.normalize.blockAveragePSD` (*psddata*, *Nav*, ****kwargs**)

perform a block average for several PSD spectra all data are used therefore the last cell used for averaging may differ in size

Parameter

psddataarray of 2D data shape (Nspectra,Nchannels)

Navnumber of channels which should be averaged

****kwargs: optional keyword argument**

roiregion of interest for the 2D array. e.g. [20,980] Nchannels = 980-20

Returns

block averaged psd spectra as numpy array with type numpy.double of shape (Nspectra , ceil(Nchannels/Nav))

utilities Module

xrayutilities utilities contains a conglomeration of useful functions which do not fit into one of the other files

`xrayutilities.utilities.maplog (inte, dynlow='config', dynhigh='config', **keyargs)`
 clips values smaller and larger as the given bounds and returns the log10 of the input array. The bounds are given as exponent with base 10 with respect to the maximum in the input array. The function is implemented in analogy to J. Stangl's matlab implementation.

Parameters

inte numpy.array, values to be cut in range

dynlow $10^{(-dynlow)}$ will be the minimum cut off

dynhigh $10^{(-dynhigh)}$ will be the maximum cut off

optional keyword arguments (NOT IMPLEMENTED):

abslow $10^{(abslow)}$ will be taken as lower boundary

abshigh $10^{(abshigh)}$ will be taken as higher boundary

Returns

numpy.array of the same shape as inte, where values smaller/larger then $10^{(-dynlow, dynhigh)}$ were replaced by $10^{(-dynlow, dynhigh)}$

Example

```
>>> lint = maplog(int, 5, 2)
```

utilities_noconf Module

xrayutilities utilities contains a conglomeration of useful functions this part of utilities does not need the config class

`xrayutilities.utilities_noconf.energy (en)`
 convert common energy names to energies in eV

so far this works with CuKa1, CuKa2, CuKa12, CuKb, MoKa1

Parameter

energy (scalar (energy in eV will be returned unchanged) or string with name of emission line)

Returns

energy in eV as float

`xrayutilities.utilities_noconf.lam2en (inp)`

converts the input energy in eV to a wavelength in Angstrom or the input wavelength in Angstrom to an energy in eV

Parameter

inp either an energy in eV or an wavelength in Angstrom

Returns

float, energy in eV or wavlength in Angstrom

Examples

```
>>> lambda = lam2en(8048)
>>> energy = lam2en(1.5406)
```

`xrayutilities.utilities_noconf.wavelength(wl)`

convert common energy names to energies in eV

so far this works with CuKa1, CuKa2, CuKa12, CuKb, MoKa1

Parameter

wlwavelength (scalar (wavelength in Angstrom will be returned unchanged) or string with name of emission line)

Returns

wavelength in Angstrom as float

Subpackages

analysis Package

analysis Package `xrayutilities.analysis` is a package for assisting with the analysis of x-ray diffraction data, mainly reciprocal space maps

Routines for obtaining line cuts from gridded reciprocal space maps are offered, with the ability to integrate the intensity perpendicular to the line cut direction.

line_cuts Module

`xrayutilities.analysis.line_cuts.fwhm_exp(pos, data)`

function to determine the full width at half maximum value of experimental data. Please check the obtained value visually (noise influences the result)

Parameter

posposition of the data points

datadata values

Returns

fwhm value (single float)

`xrayutilities.analysis.line_cuts.get_omega_scan_ang(qx, qz, intensity, omcenter, ttcenter, omrange, npoints, **kwargs)`

extracts an omega scan from a gridded reciprocal space map

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

omcenteromega-position at which the omega scan should be extracted

ttcenter2theta-position at which the omega scan should be extracted

omrangerange of the omega scan to extract

npointsnumber of points of the omega scan

****kwargs: possible keyword arguments:**

qrangeintegration range perpendicular to scan direction

Nintnumber of subscans used for the integration (optionally)

lamwavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative omega positions are returned (default: True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

om,omint omega scan coordinates and intensities (bounds=False)

om,omint,(qxb,qzb) omega scan coordinates and intensities + reciprocal space bounds of the extracted scan (bounds=True)

Example

```
>>> omcut, intcut = get_omega_scan(qx,qz,intensity,0.0,5.0,2.0,200)
```

```
xrayutilities.analysis.line_cuts.get_omega_scan_bounds_ang(omcenter, tt-
                                                         center, om-
                                                         range, npoints,
                                                         **kwargs)
```

return reciprocal space boundaries of omega scan

Parameters

omcenter omega-position at which the omega scan should be extracted

ttcenter 2theta-position at which the omega scan should be extracted

omrange range of the omega scan to extract

npoints number of points of the omega scan

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

lam wavelength for use in the conversion to angular coordinates

Returns

qx,qz reciprocal space coordinates of the omega scan boundaries

Example

```
>>> qxb,qzb = get_omega_scan_bounds_ang(1.0,4.0,2.4,240,qrange=0.1)
```

```
xrayutilities.analysis.line_cuts.get_omega_scan_q(qx, qz, intensity, qxcenter,
                                                  qzcenter, omrange, npoints,
                                                  **kwargs)
```

extracts an omega scan from a gridded reciprocal space map

Parameters

qx equidistant array of qx momentum transfer

qz equidistant array of qz momentum transfer

intensity 2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qxcenter qx-position at which the omega scan should be extracted

qzcenter qz-position at which the omega scan should be extracted

omrange range of the omega scan to extract

npoints number of points of the omega scan

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

Nint number of subscans used for the integration (optionally)

lam wavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative omega positions are returned (default: True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

om,omintomega scan coordinates and intensities (bounds=False)

om,omint,(qxb,qzb)omega scan coordinates and intensities + reciprocal space bounds of the extracted scan (bounds=True)

Example

```
>>> omcut, intcut = get_omega_scan(qx,qz,intensity,0.0,5.0,2.0,200)
```

`xrayutilities.analysis.line_cuts.get_qx_scan(qx,qz,intensity,qzpos,**kwargs)`
extract qx line scan at position qzpos from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given range along qz

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qzposposition at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrangeintegration range perpendicular to scan direction

qmin,qmaxminimum and maximum value of extracted scan axis

boundsflag to specify if the scan bounds of the extracted scan should be returned (default:False)

Returns

qx,qxintqx scan coordinates and intensities (bounds=False)

qx,qxint,(qxb,qyb)qx scan coordinates and intensities + scan bounds for plotting

Example

```
>>> qxcut,qxcut_int = get_qx_scan(qx,qz,inten,5.0,qrange=0.03)
```

`xrayutilities.analysis.line_cuts.get_qz_scan(qx,qz,intensity,qxpos,**kwargs)`
extract qz line scan at position qxpos from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given range along qx

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qxposposition at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrangeintegration range perpendicular to scan direction

qmin,qmaxminimum and maximum value of extracted scan axis

Returns

qz,qzintqz scan coordinates and intensities

Example

```
>>> qzcut, qzcut_int = get_qz_scan(qx, qz, inten, 1.5, qrange=0.03)
```

```
xrayutilities.analysis.line_cuts.get_qz_scan_int(qx, qz, intensity, qxpos,
**kwargs)
```

extracts a qz scan from a gridded reciprocal space map with integration along omega (sample rocking angle) or 2theta direction

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qxposposition at which the line scan should be extracted

****kwargs: possible keyword arguments:**

angrangeintegration range in angular direction

qmin,qmaxminimum and maximum value of extracted scan axis

boundsflag to specify if the scan bounds of the extracted scan should be returned (default:False)

intdirintegration direction ‘omega’: sample rocking angle (default) ‘2theta’: scattering angle

Returns

qz,qzintqz scan coordinates and intensities (bounds=False)

qz,qzint,(qzb,qzb)qz scan coordinates and intensities + scan bounds for plotting

Example

```
>>> qzcut, qzcut_int = get_qz_scan_int(qx, qz, inten, 5.0, omrange=0.3)
```

```
xrayutilities.analysis.line_cuts.get_radial_scan_ang(qx, qz, intensity, omcenter,
ttcenter, ttrange, npoints,
**kwargs)
```

extracts a radial scan from a gridded reciprocal space map

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

omcenterom-position at which the radial scan should be extracted

ttcentertt-position at which the radial scan should be extracted

ttrangetwo theta range of the radial scan to extract

npointsnumber of points of the radial scan

****kwargs: possible keyword arguments:**

omrangeintegration range perpendicular to scan direction

Nintnumber of subscans used for the integration (optionally)

lamwavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative two theta positions are returned (default=True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

om,tt,radintomega,two theta scan coordinates and intensities (bounds=False)

om,tt,radint,(qxb,qzb)radial scan coordinates and intensities + reciprocal space
bounds of the extracted scan (bounds=True)

Example

```
>>> omc,ttc,cut_int = get_radial_scan_ang(qx,qz,intensity,32.0,64.0,30.0,800,omrange=0.2)
```

```
xrayutilities.analysis.line_cuts.get_radial_scan_bounds_ang(omcenter,  
                                                            ttcenter,  
                                                            ttrange, npoints,  
                                                            **kwargs)
```

return reciprocal space boundaries of radial scan

Parameters

omcenterom-position at which the radial scan should be extracted

ttcentertt-position at which the radial scan should be extracted

ttrangetwo theta range of the radial scan to extract

npointsnumber of points of the radial scan

****kwargs: possible keyword arguments:**

omrangeintegration range perpendicular to scan direction

lamwavelength for use in the conversion to angular coordinates

Returns

qxrad,qzradreciprocal space boundaries of radial scan

Example

```
>>>
```

```
xrayutilities.analysis.line_cuts.get_radial_scan_q(qx, qz, intensity, qxcenter,  
                                                    qzcenter, ttrange, npoints,  
                                                    **kwargs)
```

extracts a radial scan from a gridded reciprocal space map

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qxcenterqx-position at which the radial scan should be extracted

qzcenterqz-position at which the radial scan should be extracted

ttrangetwo theta range of the radial scan to extract

npointsnumber of points of the radial scan

****kwargs: possible keyword arguments:**

omrangeintegration range perpendicular to scan direction

Nintnumber of subscans used for the integration (optionally)

lamwavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative two theta positions are returned (default=True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

om,tt,radintomega,two theta scan coordinates and intensities (bounds=False)

om,tt,radint,(qxb,qzb)radial scan coordinates and intensities + reciprocal space bounds of the extraced scan (bounds=True)

Example

```
>>> omc,ttc,cut_int = get_radial_scan_q(qx,qz,intensity,0.0,5.0,1.0,100,omrange=0.01)
```

```
xrayutilities.analysis.line_cuts.get_ttheta_scan_ang(qx, qz, intensity, omcenter,
                                                    ttcenter, ttrange, npoints,
                                                    **kwargs)
```

extracts a twotheta scan from a gridded reciprocal space map

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

omcenterom-position at which the 2theta scan should be extracted

ttcentertt-position at which the 2theta scan should be extracted

ttrangetwo theta range of the scan to extract

npointsnumber of points of the radial scan

****kwargs: possible keyword arguments:**

omrangeintegration range in omega direction

Nintnumber of subscans used for the integration (optionally)

lamwavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative two theta positions are returned (default=True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

tt,ttinttwo theta scan coordinates and intensities (bounds=False)

tt,ttint,(qxb,qzb)2theta scan coordinates and intensities + reciprocal space bounds of the extraced scan (bounds=True)

Example

```
>>> ttc,cut_int = get_ttheta_scan_ang(qx,qz,intensity,32.0,64.0,4.0,400)
```

```
xrayutilities.analysis.line_cuts.get_ttheta_scan_bounds_ang(omcenter,
                                                            ttcenter,
                                                            ttrange, npoints,
                                                            **kwargs)
```

return reciprocal space boundaries of 2theta scan

Parameters

omcenterom-position at which the 2theta scan should be extracted

ttcentertt-position at which the 2theta scan should be extracted

ttrangetwo theta range of the 2theta scan to extract

npointsnumber of points of the 2theta scan

****kwargs: possible keyword arguments:**

omrangeintegration range in omega direction

lamwavelength for use in the conversion to angular coordinates

Returns

qxtt,qzttreciprocal space boundaries of 2theta scan (bounds=False)

tt,ttint,(qxb,qzb)2theta scan coordinates and intensities + reciprocal space bounds of the extraced scan (bounds=True)

Example

```
>>>
```

```
xrayutilities.analysis.line_cuts.get_ttheta_scan_q(qx, qz, intensity, qxcenter,
                                                    qzcenter, ttrange, npoints,
                                                    **kwargs)
```

extracts a twotheta scan from a gridded reciprocal space map

Parameters

qxequidistant array of qx momentum transfer

qzequidistant array of qz momentum transfer

intensity2D array of gridded reciprocal space intensity with shape (qx.size,qz.size)

qxcenterqx-position at which the 2theta scan should be extracted

qzcenterqz-position at which the 2theta scan should be extracted

ttrangetwo theta range of the scan to extract

npointsnumber of points of the radial scan

****kwargs: possible keyword arguments:**

omrangeintegration range in omega direction

Nintnumber of subscans used for the integration (optionally)

lamwavelength for use in the conversion to angular coordinates

relativedetermines if absolute or relative two theta positions are returned (default=True)

boundsflag to specify if the scan bounds should be returned (default: False)

Returns

tt,ttinttwo theta scan coordinates and intensities (bounds=False)

om,tt,radint,(qxb,qzb)radial scan coordinates and intensities + reciprocal space bounds of the extraced scan (bounds=True)

Example

```
>>> ttc,cut_int = get_ttheta_scan_q(qx,qz,intensity,0.0,4.0,4.4,440)
```

```
xrayutilities.analysis.line_cuts.get_index(x,y,xgrid,ygrid)
```

gives the indices of the point x,y in the grid given by xgrid ygrid xgrid,ygrid must be arrays containing equidistant points

Parameters

x,ycoordinates of the point of interest (float)

xgrid,ygridgrid coordinates in x and y direction (array)

Returns

ix, iy index of the closest gridpoint (lower left) of the point (x,y)

line_cuts3d Module

`xrayutilities.analysis.line_cuts3d.get_qx_scan3d(gridder, qypos, qzpos, **kwargs)`

extract qx line scan at position y,z from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given area around this position

Parameters

gridder3d xrayutilities.Gridder3D object containing the data

qypos,qzpos position at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

qmin,qmax minimum and maximum value of extracted scan axis

Returns

qx,qxint qx scan coordinates and intensities

Example

```
>>> qxcut,qxcut_int = get_qx_scan3d(gridder,0,0,qrange=0.03)
```

`xrayutilities.analysis.line_cuts3d.get_qy_scan3d(gridder, qxpos, qzpos, **kwargs)`

extract qy line scan at position x,z from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given area around this position

Parameters

gridder3d xrayutilities.Gridder3D object containing the data

qxpos,qzpos position at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

qmin,qmax minimum and maximum value of extracted scan axis

Returns

qy,qyint qy scan coordinates and intensities

Example

```
>>> qycut,qycut_int = get_qy_scan3d(gridder,0,0,qrange=0.03)
```

`xrayutilities.analysis.line_cuts3d.get_qz_scan3d(gridder, qxpos, qypos, **kwargs)`

extract qz line scan at position x,y from a gridded reciprocal space map by taking the closest line of the intensity matrix, or summing up a given area around this position

Parameters

gridder3d xrayutilities.Gridder3D object containing the data

qxpos,qypos position at which the line scan should be extracted

****kwargs: possible keyword arguments:**

qrange integration range perpendicular to scan direction

qmin,qmax minimum and maximum value of extracted scan axis

Returns

qz,qzintqz scan coordinates and intensities

Example

```
>>> qzcut,qzcut_int = get_qz_scan3d(gridder,0,0,qrange=0.03)
```

`xrayutilities.analysis.line_cuts3d.get_index3d(x,y,z,xgrid,ygrid,zgrid)`

gives the indices of the point x,y,z in the grid given by xgrid ygrid zgrid xgrid,ygrid,zgrid must be arrays containing equidistant points

Parameters

x,y,zcoordinates of the point of interest (float)

xgrid,ygrid,zgridgrid coordinates in x,y,z direction (array)

Returns

ix,iy,izindex of the closest gridpoint (lower left) of the point (x,y,z)

misc Module miscellaneous functions helpful in the analysis and experiment

`xrayutilities.analysis.misc.getangles(peak,sur,inp)`

calculates the chi and phi angles for a given peak

Parameter

peakarray which gives hkl for the peak of interest

surhkl of the surface

inpinplane reference peak or direction

Returns

[chi,phi] for the given peak on surface sur with inplane direction inp as reference

Example

```
To get the angles for the -224 peak on a 111 surface type[chi,phi] = getangles([-2,2,4],[1,1,1],[2,2,4])
```

sample_align Module functions to help with experimental alignment during experiments, especially for experiments with linear detectors

```
xrayutilities.analysis.sample_align.area_detector_calib(angle1, angle2,
                                                         ccdimages, de-
                                                         taxis, r_i, plot=True,
                                                         cut_off=0.7, start=(0,
                                                         0, 0, 0), fix=(False,
                                                         False, False, False),
                                                         fig=None, wl=None)
```

function to calibrate the detector parameters of an area detector it determines the detector tilt possible rotations and offsets in the detector arm angles

parameters

angle1outer detector arm angle

angle2inner detector arm angle

ccdimagesimages of the ccd taken at the angles given above

detaxisdetector arm rotation axis :default: ['z+', 'y-']

r_iprimary beam direction [xyz][+-] default 'x+'

Keyword_arguments

plotflag to determine if results and intermediate results should be plotted :default: True

cut_offcut off intensity to decide if image is used for the determination or not :default: 0.7 = 70%

startsequence of start values of the fit for parameters, which can not be estimated automatically these are: tiltazimuth,tilt,detector_rotation,outerangle_offset. By default (0,0,0,0) is used.

fixfix parameters of start (default: (False,False,False,False))

figmatplotlib figure used for plotting the error :default: None (creates own figure)

wlwavelength of the experiment in Angstrom (default: config.WAVELENGTH) value does not matter here and does only affect the scaling of the error

```
xrayutilities.analysis.sample_align.area_detector_calib_hkl (sampleang,
                                                             angle1, angle2,
                                                             ccdimages, hkls,
                                                             experiment, material,
                                                             detaxis, r_i, plot=True,
                                                             cut_off=0.1,
                                                             start=(0, 0, 0,
                                                             0, 0, 0, 'config'),
                                                             fix=(False, False,
                                                             False, False,
                                                             False, False),
                                                             fig=None)
```

function to calibrate the detector parameters of an area detector it determines the detector tilt possible rotations and offsets in the detector arm angles

in this variant not only scans through the primary beam but also scans at a set of symmetric reflections can be used for the detector parameter determination. for this not only the detector parameters but in addition the sample orientation and wavelength need to be fit.

parameters

sampleangsample rocking angle (needed to align the reflections (same rotation direction as inner detector rotation)) other sample angle are not allowed to be changed during the scans

angle1outer detector arm angle

angle2inner detector arm angle

ccdimagesimages of the ccd taken at the angles given above

hklsarray/list of hkl values for every image

materialmaterial used as reference crystal

detaxisdetector arm rotation axis :default: ['z+', 'y-']

r_iprimary beam direction [xyz][+-] default 'x+'

Keyword_arguments

plotflag to determine if results and intermediate results should be plotted :default: True

cut_offcut off intensity to decide if image is used for the determination or not :default: 0.7 = 70%

startsequence of start values of the fit for parameters, which can not be estimated automatically these are: tiltazimuth,tilt,detector_rotation,outerangle_offset,stilt,stazimuth, wavelength. By default (0,0,0,0,0,0,'config') is used.

fixfix parameters of start (default: (False,False,False,False,False,False,False))

figmatplotlib figure used for plotting the error :default: None (creates own figure)

`xrayutilities.analysis.sample_align.fit_bragg_peak` (*om, tt, psd, omalign, ttalign, exphrd, frange=(0.03, 0.03), plot=True*)

helper function to determine the Bragg peak position in a reciprocal space map used to obtain the position needed for correction of the data. the determination is done by fitting a two dimensional Gaussian (`xrayutilities.math.Gauss2d`)

PLEASE ALWAYS CHECK THE RESULT CAREFULLY!

Parameter

om,ttangular coordinates of the measurement (numpy.ndarray) either with size of psd or of psd.shape[0]

psdintensity values needed for fitting

omalignaligned omega value, used as first guess in the fit

ttalignaligned two theta values used as first guess in the fit these values are also used to set the range for the fit: the peak should be within +/-frangeAA⁻¹ of those values

exphrdexperiment class used for the conversion between angular and reciprocal space.

frangedata range used for the fit in both directions (see above for details default:(0.03,0.03) unit: AA⁻¹)

plotif True (default) function will plot the result of the fit in comparison with the measurement.

Returns

Omfit,ttfit,params,covariance fitted angular values, and the fit parameters (of the Gaussian) as well as their errors

`xrayutilities.analysis.sample_align.linear_detector_calib` (*angle, mca_spectra, **keyargs*)

function to calibrate the detector distance/channel per degrees for a straight linear detector mounted on a detector arm

parameters

anglearray of angles in degree of measured detector spectra

mca_spectracorresponding detector spectra :(shape: (len(angle),Nchannels))

****keyargs** passed to `psd_chdeg` function used for the modelling, additional options are:

r_iprimary beam direction as vector [xyz][+-]; default: 'y+'

detaxisdetector arm rotation axis [xyz][+-] e.g. 'x+'; default: 'x+'

selected options from psd_chdeg:

plotflag to specify if a visualization of the fit should be done

usetiltwhether to use model considering a detector tilt (deviation angle of the pixel direction from orthogonal to the primary beam) (default: True)

Note: Note: see help of psd_chdeg for more options

returns

pixelwidth (at one meter distance) , center_channel[, detector_tilt]

Note: Note: $L/\text{pixelwidth} \cdot \pi/180 \approx \text{channel/degree}$, with the sample detector distance L

pixelwidth is negative in case the hit channel number decreases upon an increase of the detector angle
The function also prints out how a linear detector can be initialized using the results obtained from this calibration. Carefully check the results

`xrayutilities.analysis.sample_align.miscut_calc(phi, aomega, zeros=None, plot=True, omega0=None)`

function to calculate the miscut direction and miscut angle of a sample by fitting a sinusoidal function to the variation of the aligned omega values of more than two reflections. The function can also be used to fit reflectivity alignment values in various azimuths.

Parameters

phiazimuths in which the reflection was aligned (deg)

aomegaaligned omega values (deg)

zeros(optional) angles at which surface is parallel to the beam (deg). For the analysis the angles (aomega-zeros) are used.

plotflag to specify if a visualization of the fit is wanted. :default: True

omega0if specified the nominal value of the reflection is not included as fit parameter, but is fixed to the specified value. This value is MANDATORY if ONLY TWO AZIMUTHs are given.

Returns

[omega0,phi0,miscut]

list with fitted values for

omega0the omega value of the reflection should be close to the nominal one

phi0the azimuth in which the primary beam looks upstairs

miscutamplitude of the sinusoidal variation == miscut angle

`xrayutilities.analysis.sample_align.psd_chdeg(angles, channels, stdev=None, usetilt=True, plot=True, datap='kx', modelline='r-', modeltilt='b-', fignum=None, mlabel='fit', mtilt-label='fit w/tilt', dlabel='data', figtitle=True)`

function to determine the channels per degree using a linear fit of the function $nchannel = center_ch + chdeg \cdot \tan(angles)$ or the equivalent including a detector tilt

Parameters

anglesdetector angles for which the position of the beam was measured

channelsdetector channels where the beam was found

keyword arguments:

stdevstandard deviation of the beam position

plotflag to specify if a visualization of the fit should be done

usetiltwhether to use model considering a detector tilt (deviation angle of the pixel direction from orthogonal to the primary beam) (default: True)

dataplotformat of data points

modellineplotformat of modelline

modeltiltplotformat of modeltilt

fignumfigure number to use for the plot

mlabellabel of the model w/o tilt to be used in the plot

mtiltlabellabel of the model with tilt to be used in the plot

dlabellabel of the data line to be used in the plot

figtitleboolean to tell if the figure title should show the fit parameters

Returns

(pixelwidth,centerch,tilt)

Pixelwidth the width of one detector channel @ 1m distance, which is negative in case the hit channel number decreases upon an increase of the detector angle.

Centerch center channel of the detector

Tilt tilt of the detector from perpendicular to the beam (will be zero in case of usetilt=False)

Note: Note: $L/\text{pixelwidth} \cdot \pi/180 = \text{channel/degree}$ for large detector distance with the sample detector distance L

`xrayutilities.analysis.sample_align.psd_refl_align` (*primarybeam, angles, channels, plot=True*)

function which calculates the angle at which the sample is parallel to the beam from various angles and detector channels from the reflected beam. The function can be used during the half beam alignment with a linear detector.

Parameters

primarybeamprimary beam channel number

angleslist or numpy.array with angles

channelslist or numpy.array with corresponding detector channels

plotflag to specify if a visualization of the fit is wanted :default: True

Returns

omegaangle at which the sample is parallel to the beam

Example

```
>>> psd_refl_align(500, [0, 0.1, 0.2, 0.3], [550, 600, 640, 700])
```

io Package

io Package

edf Module

```
class xrayutilities.io.edf.EDFDirectory (datapath, ext='edf', **keyargs)
```

Bases: object

Parses a directory for EDF files, which can be stored to a HDF5 file for further usage

```
Save2HDF5 (h5, group='', comp=True)
```

Saves the data stored in the EDF files in the specified directory in a HDF5 file as a HDF5 arrays in a subgroup. By default the data is stored in a group given by the foldername - this can be changed by passing the name of a target group or a path to the target group via the “group” keyword argument.

required arguments. :h5: a HDF5 file object

optional keyword arguments: :group: group where to store the data (defaults to pathname if group is empty string) :comp: activate compression - true by default

```
class xrayutilities.io.edf.EDFFile (fname, nxkey='Dim_1', nykey='Dim_2',
                                   dtkey='DataType', path='', header=True)
```

Bases: object

```
ReadData ()
```

Read the CCD data into the .data object this function is called by the initialization

```
Save2HDF5 (h5, group='/', comp=True)
```

Saves the data stored in the EDF file in a HDF5 file as a HDF5 array. By default the data is stored in the root group of the HDF5 file - this can be changed by passing the name of a target group or a path to the target group via the “group” keyword argument.

required arguments. :h5: a HDF5 file object

optional keyword arguments: :group: group where to store the data (default to the root of the file) :comp: activate compression - true by default

imagereader Module

```
class xrayutilities.io.imagereader.ImageReader (nop1, nop2, hdrlen=0, flatfield=None,
                                                darkfield=None, dtype=<type
                                                'numpy.int16'>, byte_swap=False)
```

Bases: object

parse CCD frames in the form of tiffs or binary data (*.bin) to numpy arrays. ignore the header since it seems to contain no useful data

The routine was tested so far withRoperScientific files with 4096x4096 pixels created at Hasylab Hamburg, which save an 16bit integer per point. Perkin Elmer images created at Hasylab Hamburg with 2048x2048 pixels.

```
readImage (filename)
```

read image file and correct for dark- and flatfield in case the necessary data are available.

returned data = ((image data)-(darkfield))/flatfield*average(flatfield)

Parameter

filenamefilename of the image to be read. so far only single filenames are supported.

The data might be compressed. supported extensions: .tiff, .bin and .bin.xz

```
class xrayutilities.io.imagereader.PerkinElmer (**keyargs)
```

Bases: `xrayutilities.io.imagereader.ImageReader`

parse PerkinElmer CCD frames (*.bin) to numpy arrays Ignore the header since it seems to contain no useful data

The routine was tested only for files with 2048x2048 pixel images created at Hasylab Hamburg which save an 32bit float per point.

```
class xrayutilities.io.imagereader.RoperCCD (**keyargs)
```

Bases: `xrayutilities.io.imagereader.ImageReader`

parse RoperScientific CCD frames (*.bin) to numpy arrays Ignore the header since it seems to contain no useful data

The routine was tested only for files with 4096x4096 pixel images created at HasyLab Hamburg which save an 16bit integer per point.

panalytical_xml Module Panalytical XML (www.XRDML.com) data file parser

based on the native python xml.dom.minidom module. want to keep the number of dependancies as small as possible

class xrayutilities.io.panalytical_xml.XRDMLFile (*fname*)

Bases: object

class to handle XRDML data files. The class is supplied with a file name and uses the XRDMLScan class to parse the xrdMeasurement in the file

class xrayutilities.io.panalytical_xml.XRDMLMeasurement (*measurement*)

Bases: object

class to handle scans in a XRDML datafile

xrayutilities.io.panalytical_xml.getOmPixel (*omraw, ttraw*)

function to reshape the Omega values into a form needed for further treatment with xrayutilities

xrayutilities.io.panalytical_xml.getxrdml_map (*filetemplate, scannrs=None, path='.',
roi=None*)

parses multiple XRDML file and concatenates the results for parsing the xrayutilities.io.XRDMLFile class is used. The function can be used for parsing maps measured with the PIXCel and point detector.

Parameter

filetemplatetemplate string for the file names, can contain a %d which is replaced by the scan number or be a list of filenames

scannrsint or list of scan numbers

pathcommon path to the filenames

roiregion of interest for the PIXCel detector, for other measurements this is not useful!

Returns

om,tt,psdas flattened numpy arrays

Example

```
>>> om,tt,psd = xrayutilities.io.getxrdml_map("samplename_%d.xrdml", [1,2],path="./data")
```

radicon Module python module for converting radicon data to HDF5

xrayutilities.io.radicon.hst2hdf5 (*h5, hstfile, nofchannels, h5path='/', hstpath='.'*)

Converts a HST file to an HDF5 file.

Required input arguments:

h5HDF5 object where to store the data

hstfilename of the HST file

nofchannelsnumber of channels

optional input arguments:

h5pathPath in the HDF5 file where to store the data

hstpathpath where the HST file is located (default is the current working directory)

xrayutilities.io.radicon.rad2hdf5 (*h5, rdcfile, h5path='/', rdcpath='.'*)

Converts a RDC file to an HDF5 file.

Required input arguments:

h5HDF5 object where to store the data

rdcfilename of the RDC file

optional input arguments:

h5pathPath in the HDF5 file where to store the data (default to root)

rdcpathpath where the RDC file is located (default is the current working directory)

`xrayutilities.io.radicon.selecthst` (*et_limit*, *mca_info*, *mca_array*)

Select histograms from the complete set of recorded MCA data and stores it into a new numpy array. The selection is done due to a exposure time limit. Spectra below this limit are ignored.

required input arguments:

et_limitexposure time limit

mca_infopytables table with the exposure data

mca_arrayarray with all the MCA spectra

return value:a numpy array with the selected mca spectra of shape (hstnr,channels).

rotanode_alignment Module parser for the alignment log file of the rotating anode

class `xrayutilities.io.rotanode_alignment.RA_Alignment` (*filename*)

Bases: object

class to parse the data file created by the alignment routine (tpalign) at the rotating anode spec installation

this routine does an iterative alignment procedure and saves the center of mass values were it moves after each scan. It iterates between two different peaks and iteratively aligns at each peak between two different motors (om/chi at symmetric peaks, om/phi at asymmetric peaks)

Parse ()

parser to read the alignment log and obtain the aligned values at every iteration.

get (*key*)

keys ()

returns a list of keys for which aligned values were parsed

plot (*pname*)

function to plot the alignment history for a given peak

Parameters

pnamepeakname for which the alignment should be plotted

seifert Module a set of routines to convert Seifert ASCII files to HDF5 in fact there exist two possibilities how the data is stored (depending on the use detector):

1. as a simple line scan (using the point detector)
2. as a map using the PSD

In the first case the data ist stored

class `xrayutilities.io.seifert.SeifertHeader`

Bases: object

save_h5_attribs (*obj*)

class `xrayutilities.io.seifert.SeifertMultiScan` (*filename*, *m_scan*, *m2*, *path=None*)

Bases: object

dump2hdf5 (*h5, iname='INT', group='/'*)

Saves the content of a multi-scan file to a HDF5 file. By default the data is stored in the root group of the file. To save data somewhere else the keyword argument “group” must be used.

required arguments:

h5a HDF5 file object

optional keyword arguments:

inamename for the intensity matrix

grouppath to the HDF5 group where to store the data

dump2mlab (*fname, *args*)

Store the data in a matlab file.

parse ()

class `xrayutilities.io.seifert.SeifertScan` (*filename, path=None*)

Bases: `object`

dump2h5 (*h5, *args, **keyargs*)

Save the data stored in the Seifert ASCII file to a HDF5 file.

required input arguments:

h5HDF5 file object

optional arguments:

names to use to store the motors. The first must be the name for the intensity array. The number of names must be equal to the second element of the shape of the data object.

optional keyword arguments:

groupHDF5 group object where to store the data.

dump2mlab (*fname, *args*)

Save the data from a Seifert scan to a matlab file.

required input arguments:

fnamename of the matlab file

optional position arguments:

names to use to store the motors. The first must be the name for the intensity array. The number of names must be equal to the second element of the shape of the data object.

parse ()

`xrayutilities.io.seifert.getSeifert_map` (*filetemplate, scannrs=None, path='.', scantype='map', Nchannels=1280*)

parses multiple Seifert *.nja files and concatenates the results. for parsing the `xrayutilities.io.SeifertMultiScan` class is used. The function can be used for parsing maps measured with the Meteor1D and point detector.

Parameter

filetemplatetemplate string for the file names, can contain a %d which is replaced by the scan number or be a list of filenames

scannrsint or list of scan numbers

pathcommon path to the filenames

scantypetype of datafile: “map”: reciprocal space map measured with a regular Seifert job “tsk”: MCA spectra measured using the TaskInterpreter

Nchannelsnumber of channels of the MCA (needed for “tsk” measurements)

Returns

om,tt,psdas flattened numpy arrays

Example

```
>>> om,tt,psd = xrayutilities.io.getSeifert_map("samplename_%d.xrdml",[1,2],path="./data")
```

`xrayutilities.io.seifert.repair_key(key)`

Repair a key string in the sense that the string is changed in a way that it can be used as a valid Python identifier. For that purpose all blanks within the string will be replaced by `_` and leading numbers get an preceding `_`.

spec Module a threaded class for observing a SPEC data file

Motivation

SPEC files can become quite large. Therefore, subsequently reading the entire file to extract a single scan is a quite cumbersome procedure. This module is a proof of concept code to write a file observer starting a reread of the file starting from a stored offset (last known scan position)

class `xrayutilities.io.spec.SPECCmdLine(n, prompt, cmdl, out)`

Bases: `object`

Save2HDF5 (*h5, **keyargs*)

class `xrayutilities.io.spec.SPECFile(filename, path='')`

Bases: `object`

This class represents a single SPEC file. The class provides methodes for updateing an already opened file which makes it particular interesting for interactive use.

Parse()

Parses the file from the starting at `last_offset` and adding found scans to the scan list.

Save2HDF5 (*h5f, comp=True*)

Save the entire file in an HDF5 file. For that purpose a group is set up in the root group of the file with the name of the file without extension and leading path. If the method is called after an previous update only the scans not written to the file meanwhile are saved.

required arguments:

h5fa HDF5 file object or its filename

optional keyword arguments:

compactivate compression - true by default

Update()

reread the file and add newly added files. The parsing starts at the data offset of the last scan gathered during the last parsing run.

class `xrayutilities.io.spec.SPECLog(filename, prompt, path='')`

Bases: `object`

Parse()

Update()

class `xrayutilities.io.spec.SPECMCA(nchan, roistart, roistop)`

Bases: `object`

SPECMCA - represents an MCA object in a SPEC file. This class is an abstract class not itended for being used directly. Instead use one of the derived classes `SPECMCAFile` or `SPECMCAInline`.

class `xrayutilities.io.spec.SPECMCAFile`

Bases: `xrayutilities.io.spec.SPECMCA`

ReadData()

class xrayutilities.io.spec.SPECMCAInline

Bases: xrayutilities.io.spec.SPECMCA

ReadData ()

class xrayutilities.io.spec.SPECScan(*name, scannr, command, date, time, itime, col-names, hoffset, doffset, fid, imopnames, imopvalues, scan_status*)

Bases: object

Represents a single SPEC scan.

ClearData ()

Delete the data stored in a scan after it is no longer used.

ReadData ()

Set the data attribute of the scan class.

Save2HDF5 (*h5f, group='/', title='', desc='', optattrs={}, comp=True*)

Save a SPEC scan to an HDF5 file. The method creates a group with the name of the scan and stores the data there as a table object with name “data”. By default the scan group is created under the root group of the HDF5 file. The title of the scan group is usually the scan command. Metadata of the scan are stored as attributes to the scan group. Additional custom attributes to the scan group can be passed as a dictionary via the *optattrs* keyword argument.

input arguments:

h5fa HDF5 file object or its filename

optional keyword arguments:

groupname or group object of the HDF5 group where to store the data

titlea string with the title for the data, defaults to the name of scan if empty

desca string with the description of the data, defaults to the scan command if empty

optattrsa dictionary with optional attributes to store for the data

compactivate compression - true by default

SetMCAParams (*mca_column_format, mca_channels, mca_start, mca_stop*)

Set the parameters used to save the MCA data to the file. This method calculates the number of lines used to store the MCA data from the number of columns and the

required input arguments:

mca_column_formatnumber of columns used to save the data

mca_channelsnumber of MCA channels stored

mca_startfirst channel that is stored

mca_stoplast channel that is stored

plot (**args, **keyargs*)

Plot scan data to a matplotlib figure. If *newfig=True* a new figure instance will be created. If *logy=True* (default is False) the y-axis will be plotted with a logarithmic scale.

Parameters

***args: arguments for the plot: first argument is the name of x-value column**the following pairs of arguments are the y-value names and plot styles allowed are 3,5,7,... number of arguments

****keyargs:**

newfigif True a new figure instance will be created otherwise an existing one will be used

logyif True a semilogy plot will be done

`xrayutilities.io.spec.geth5_scan(h5f, scans, *args, **kwargs)`

function to obtain the angular coordinates as well as intensity values saved in an HDF5 file, which was created from a spec file by the Save2HDF5 method. Especially usefull for reciprocal space map measurements.

further more it is possible to obtain even more positions from the data file if more than two string arguments with its names are given

Parameters

h5file object of a HDF5 file opened using pytables or its filename

scans number of the scans of the reciprocal space map (int,tuple or list)

***args**: names of the motors (optional) (strings) to read reciprocal space maps measured in coplanar diffraction give: :omname: e.g. name of the omega motor (or its equivalent) :ttname: e.g. name of the two theta motor (or its equivalent)

****kwargs (optional):**

samplename string with the hdf5-group containing the scan data if omitted the first child node of h5f.root will be used

Returns

MAP

or

[ang1,ang2,...],MAP: angular positions of the center channel of the position sensitive detector (numpy.ndarray 1D) together with all the data values as stored in the data file (includes the intensities e.g. MAP['MCA']).

Example

```
>>> [om,tt],MAP = xu.io.geth5_scan(h5file,36,'omega','gamma')
```

spectra Module module to handle spectra data

class xrayutilities.io.spectra.SPECTRAFile (filename, mcatmp=None, mcastart=None, mcastop=None)

Bases: object

Represents a SPECTRA data file. The file is read during the Constructor call. This class should work for data stored at beamlines P08 and BW2 at HASYLAB.

Required constructor arguments:

filename a string with the name of the SPECTRA file

Optional keyword arguments:

mcatmp template for the MCA files

mcastart,mcastop start and stop index for the MCA files, if not given, the class tries to determine the start and stop index automatically.

Read()

Read the data from the file.

ReadMCA()

Save2HDF5 (h5file, name, group='/', description='SPECTRA scan', mcaname='MCA')

Saves the scan to an HDF5 file. The scan is saved to a seperate group of name "name". h5file is either a string for the file name or a HDF5 file object. If the mca attribute is not None mca data will be stored to an chunked array of with name mcaname.

required input arguments:

h5file string or HDF5 file object

namename of the group where to store the data

optional keyword arguments:

grouproot group where to store the data

descriptionstring with a description of the scan

Return value: The method returns None in the case of everything went fine, True otherwise.

class `xrayutilities.io.spectra.SPECTRAFileComments`

Bases: dict

Class that describes the comments in the header of a SPECTRA file. The different comments are accessible via the comment keys.

class `xrayutilities.io.spectra.SPECTRAFileData`

Bases: object

append (*col*)

class `xrayutilities.io.spectra.SPECTRAFileDataColumn` (*index, name, unit, type*)

Bases: object

class `xrayutilities.io.spectra.SPECTRAFileParameters`

Bases: dict

class `xrayutilities.io.spectra.Spectra` (*data_dir*)

Bases: object

abs_corr (*data, f, **keyargs*)

Perform absorber correction. Data can be either a 1 dimensional data (point detector) or a 2D MCA array. In the case of an array the data array should be of shape (N,NChannels) where N is the number of points in the scan an NChannels the number of channels of the MCA. The absorber values are passed to the function as a 1D array of N elements.

By default the absorber values are taken form a global variable stored in the module called `_absorber_factors`. Despite this, costume values can be passed via optional keyword arguments.

required input arguments:

mcamatrix with the MCA data

ffilter values along the scan

optional keyword arguments:

ffcustome filter factors

return value:Array with the same shape as mca with the corrected MCA data.

recarray2hdf5 (*h5g, rec, name, desc*)

Save a record array in an HDF5 file. A pytables table object is used to store the data.

required input arguments:

h5gHDF5 group object or path

recrecord array

namename of the table in the file

descdescription of the table in the file

return value:

taba HDF5 table object

set_abs_factors (*ff*)

Set the global absorber factors in the module.

spectra2hdf5 (*dir, fname, mcatemp, name='', desc='SPECTRA data'*)

Convert SPECTRA scan data to a HDF5 format.

required input arguments:

dir directory where the scan is stored
fname name of the SPECTRA data file
mcatemp template for the MCA file names

optional keyword arguments:

name optional name under which to save the data if empty the basename of the filename will be used
desc optional description of the scan

`xrayutilities.io.spectra.get_spectra_files (dirname)`

Return a list of spectra files within a directory.

required input arguments:

dirname name of the directory to search

return values: list with filenames

`xrayutilities.io.spectra.get_h5_spectra_map (h5file, scans, *args, **kwargs)`

function to obtain the omega and twotheta as well as intensity values for a reciprocal space map saved in an HDF5 file, which was created from a spectra file by the Save2HDF5 method.

further more it is possible to obtain even more positions from the data file if more than two string arguments with its names are given

Parameters

h5f file object of a HDF5 file opened using pytables
scans number of the scans of the reciprocal space map (int, tuple or list)

***args:** arbitrary number of motor names (strings)

om name of the omega motor (or its equivalent)
tt name of the two theta motor (or its equivalent)

****kwargs (optional):**

mca name of the mca data (if available) otherwise None (default: "MCA")
sample name string with the hdf5-group containing the scan data if omitted the first child node of h5f.root will be used to determine the sample name

Returns

[ang1, ang2, ...], MAP: angular positions of the center channel of the position sensitive detector (numpy.ndarray 1D) together with all the data values as stored in the data file (includes the intensities e.g. MAP['MCA']).

`xrayutilities.io.spectra.read_data (fname)`

Read a spectra data file (a file with now MCA data).

required input arguments:

fname name of the file to read

return values: (data, hdr)

data numpy record array where the keys are the column names
hdr dictionary with header information

`xrayutilities.io.spectra.read_mca (fname)`

Read a single SPECTRA MCA file.

required input arguments:

fname name of the file to read

return value:

data a numpy array with the MCA data

`xrayutilities.io.spectra.read_mca_dir (dirname, filetemp, sort=True)`

Read all MCA files within a directory

`xrayutilities.io.spectra.read_mcas (ftemp, cntstart, cntstop)`

Read MCA data from a SPECTRA MCA directory. The filename is passed as a generic

materials Package

materials Package

_create_database Module script to create the HDF5 database from the raw data of XOP this file is only needed for administration

_create_database_alt Module script to create the HDF5 database from the raw data of XOP this file is only needed for administration

cif Module

class `xrayutilities.materials.cif.CIFFile (filename)`

Bases: object

class for parsing CIF (Crystallographic Information File) files. The class aims to provide an additional way of creating material classes instead of manual entering of the information the lattice constants and unit cell structure are parsed from the CIF file

Lattice ()

returns a lattice object with the structure from the CIF file

Parse ()

function to parse a CIF file. The function reads the space group symmetry operations and the basic atom positions as well as the lattice constants and unit cell angles

SymStruct ()

function to obtain the list of different atom positions in the unit cell for the different types of atoms. The data are obtained from the data parsed from the CIF file.

database Module module to handle access to the optical parameters database

class `xrayutilities.materials.database.DataBase (fname)`

Bases: object

Close ()

Close an opened database file.

Create (dbname, dbdesc)

Creates a new database. If the database file already exists its content is deleted.

required input arguments:

dbname name of the database

dbdesc a short description of the database

CreateMaterial (name, description)

This method creates a new material. If the material group already exists the procedure is aborted.

required input arguments:

namea string with the name of the material

descriptiona string with a description of the material

GetF0 (*q*)

Obtain the f0 scattering factor component for a particular momentum transfer *q*.

required input argument:

qsingle float value or numpy array

GetF1 (*en*)

Return the second, energy dependent, real part of the scattering factor for a certain energy *en*.

required input arguments:

enfloat or numpy array with the energy

GetF2 (*en*)

Return the imaginary part of the scattering factor for a certain energy *en*.

required input arguments:

enfloat or numpy array with the energy

Open (*mode*='r')

Open an existing database file.

SetF0 (*parameters*)

Save f0 fit parameters for the set material. The fit parameters are stored in the following order:

c, a1, b1,, a4, b4

required input argument:

parameterslist or numpy array with the fit parameters

SetF1 (*en, f1*)

Set f1 tabels values for the active material.

required input arguments:

enlist or numpy array with energy in (eV)

f1list or numpy array with f1 values

SetF2 (*en, f2*)

Set f2 tabels values for the active material.

required input arguments:

enlist or numpy array with energy in (eV)

f2list or numpy array with f2 values

SetMaterial (*name*)

Set a particular material in the database as the actual material. All operations like setting and getting optical constants are done for this particular material.

required input arguments:

namestring with the name of the material

SetWeight (*weight*)

Save weight of the element as float

required input argument:

weightatomic standard weight of the element (float)

`xrayutilities.materials.database.add_f0_from_intertab(db, itabfile)`

Read f0 data from international tables of crystallography and add it to the database.

```
xrayutilities.materials.database.add_f0_from_xop(db, xopfile)
    Read f0 data from f0_xop.dat and add it to the database.

xrayutilities.materials.database.add_f1f2_from_ascii_file(db, asciifile, element)
    Read f1 and f2 data for specific element from ASCII file (3 columns) and save it to the database.

xrayutilities.materials.database.add_f1f2_from_henkedb(db, henkefile)
    Read f1 and f2 data from Henke database and add it to the database.

xrayutilities.materials.database.add_f1f2_from_kissel(db, kisselfile)
    Read f1 and f2 data from Henke database and add it to the database.

xrayutilities.materials.database.add_mass_from_NIST(db, nistfile)
    Read atoms standard mass and save it to the database.

xrayutilities.materials.database.init_material_db(db)
```

elements Module

lattice Module module handling crystal lattice structures

```
class xrayutilities.materials.lattice.Atom(name, num)
    Bases: object

    f(q, en='config')
        function to calculate the atomic structure factor F

        Parameter

            qmomentum transfer

            enenergy for which F should be calculated, if omitted the value from the xrayutilities
            configuration is used

        Returns

            f(float)

    f0(q)
    f1(en='config')
    f2(en='config')

xrayutilities.materials.lattice.BCCLattice(aa, a)
xrayutilities.materials.lattice.BCTLattice(aa, a, c)
xrayutilities.materials.lattice.BaddeleyiteLattice(aa, ab, a, b, c, beta, deg=True)
xrayutilities.materials.lattice.CuMnAsLattice(aa, ab, ac, a, b, c)
xrayutilities.materials.lattice.CubicFm3mBaF2(aa, ab, a)
xrayutilities.materials.lattice.CubicLattice(a)
    Returns a Lattice object representing a simple cubic lattice.

    required input arguments:

        alattice parameter

    return value:an instance of Lattice class

xrayutilities.materials.lattice.DiamondLattice(aa, a)
xrayutilities.materials.lattice.FCCLattice(aa, a)
xrayutilities.materials.lattice.GeneralPrimitiveLattice(a, b, c, alpha, beta, gamma)
```



```
xrayutilities.materials.lattice.HCPLattice(aa, a, c)
xrayutilities.materials.lattice.Hexagonal3CLattice(aa, ab, a, c)
xrayutilities.materials.lattice.Hexagonal4HLattice(aa, ab, a, c, u=0.1875,
                                                    v1=0.25, v2=0.4375)
xrayutilities.materials.lattice.Hexagonal6HLattice(aa, ab, a, c)
```

```
class xrayutilities.materials.lattice.Lattice(a1, a2, a3, base=None)
```

Bases: object

class Lattice: This object represents a Bravais lattice. A lattice consists of a base

ApplyStrain (*eps*)

Applies a certain strain on a lattice. The result is a change in the base vectors.

required input arguments:

epsa 3x3 matrix independent strain components

GetPoint (**args*)

determine lattice points with indices given in the argument

Examples

```
>>> xu.materials.Si.lattice.GetPoint(0,0,4)
array([ 0.      ,  0.      , 21.72416])
```

or

```
>>> xu.materials.Si.lattice.GetPoint((1,1,1))
array([ 5.43104,  5.43104,  5.43104])
```

ReciprocalLattice ()

UnitCellVolume ()

function to calculate the unit cell volume of a lattice (angstrom³)

```
class xrayutilities.materials.lattice.LatticeBase(*args, **keyargs)
```

Bases: list

The LatticeBase class implements a container for a set of points that form the base of a crystal lattice. An instance of this class can be treated as a simple container object.

append (*atom, pos, occ=1.0, b=0.0*)

add new Atom to the lattice base

Parameter

atom atom object to be added

pos position of the atom

occ occupancy (default=1.0)

b b-factor of the atom used as $\exp(-b \cdot q^2 / (4 \cdot \pi))$ to reduce the intensity of this atom (only used in case of temp=0 in StructureFactor and chi calculation)

```
xrayutilities.materials.lattice.NaumanniteLattice(aa, ab, a, b, c)
xrayutilities.materials.lattice.PerovskiteTypeRhombohedral(aa, ab, ac, a, ang)
xrayutilities.materials.lattice.QuartzLattice(aa, ab, a, b, c)
xrayutilities.materials.lattice.RockSaltLattice(aa, ab, a)
xrayutilities.materials.lattice.RockSalt_Cubic_Lattice(aa, ab, a)
xrayutilities.materials.lattice.RutileLattice(aa, ab, a, c, u)
xrayutilities.materials.lattice.TetragonalIndiumLattice(aa, a, c)
```

```
xrayutilities.materials.lattice.TetragonalTinLattice (aa, a, c)
xrayutilities.materials.lattice.TrigonalR3mh (aa, a, c)
xrayutilities.materials.lattice.WurtziteLattice (aa, ab, a, c, u=0.375, biso=0.0)
xrayutilities.materials.lattice.ZincBlendeLattice (aa, ab, a)
```

material Module class module implements a certain material

class xrayutilities.materials.material.**Alloy** (matA, matB, x)

Bases: xrayutilities.materials.material.**Material**

RelaxationTriangle (hkl, sub, exp)

function which returns the relaxation triangle for a Alloy of given composition. Reciprocal space coordinates are calculated using the user-supplied experimental class

Parameter

hkl Miller Indices

sub substrate material or lattice constant (Instance of Material class or float)

exp Experiment class from which the Transformation object and ndir are needed

Returns

qy,qz reciprocal space coordinates of the corners of the relaxation triangle

lattice_const_AB (latA, latB, x)

method to set the composition of the Alloy. x is the atomic fraction of the component B

x

xrayutilities.materials.material.**Cij2Cijkl** (cij)

Converts the elastic constants matrix (tensor of rank 2) to the full rank 4 cijkl tensor.

required input arguments:

cij(6,6) cij matrix as a numpy array

return value:

cijkl(3,3,3,3) cijkl tensor as numpy array

xrayutilities.materials.material.**Cijkl2Cij** (cijkl)

Converts the full rank 4 tensor of the elastic constants to the (6,6) matrix of elastic constants.

required input arguments:

cijkl(3,3,3,3) cijkl tensor as numpy array

return value:

cij(6,6) cij matrix as a numpy array

class xrayutilities.materials.material.**CubicAlloy** (matA, matB, x)

Bases: xrayutilities.materials.material.**Alloy**

ContentBasym (q_inp, q_perp, hkl, sur)

function that determines the content of B in the alloy from the reciprocal space position of an asymmetric peak and also sets the content in the current material

Parameter

q_inp inplane peak position of reflection hkl of the alloy in reciprocal space

q_perp perpendicular peak position of the reflection hkl of the alloy in reciprocal space

hkl Miller indices of the measured asymmetric reflection

sur Miller indices of the surface (determines the perpendicular direction)

Returns

content, [**a_inplane**, **a_perp**, **a_bulk_perp**(**x**), **eps_inplane**, **eps_perp**] : the content of B in the alloy determined from the input variables and the lattice constants calculated from the reciprocal space positions as well as the strain (**eps**) of the layer

ContentBsym (*q_perp, hkl, inpr, asub, relax*)

function that determines the content of B in the alloy from the reciprocal space position of a symmetric peak. As an additional input the substrate's lattice parameter and the degree of relaxation must be given

Parameter

q_perp perpendicular peak position of the reflection **hkl** of the alloy in reciprocal space

hkl Miller indices of the measured symmetric reflection (also defines the surface normal)

inpr Miller indices of a Bragg peak defining the inplane reference direction

asub substrate lattice constant

relax degree of relaxation (needed to obtain the content from symmetric reciprocal space position)

Returns

content the content of B in the alloy determined from the input variables

`xrayutilities.materials.material.CubicElasticTensor` (*c11, c12, c44*)

Assemble the 6x6 matrix of elastic constants for a cubic material from the three independent components of a cubic crystal

Parameter

c11, c12, c44 independent components of the elastic tensor of cubic materials

Returns

6x6 matrix with elastic constants

`xrayutilities.materials.material.GeneralUC` (*a=4, b=4, c=4, alpha=90, beta=90, gamma=90, name='General'*)

general material with primitive unit cell but possibility for different a,b,c and alpha,beta,gamma

Parameters

a, b, c unit cell extensions (Angstrom)

alpha angle between unit cell vectors b, c

beta angle between unit cell vectors a, c

gamma angle between unit cell vectors a, b

returns a Material object with the specified properties

`xrayutilities.materials.material.HexagonalElasticTensor` (*c11, c12, c13, c33, c44*)

Assemble the 6x6 matrix of elastic constants for a hexagonal material from the five independent components of a hexagonal crystal

Parameter

c11, c12, c13, c33, c44 independent components of the elastic tensor of a hexagonal material

Returns

6x6 matrix with elastic constants

class xrayutilities.materials.material.**Material** (*name, lat, cij=None, thetaDebye=None*)

Bases: object

ApplyStrain (*strain, **keyargs*)

B

GetMismatch (*mat*)

Calculate the mismatch strain between the material and a second material

Q (**hkl*)

Return the Q-space position for a certain material.

required input arguments:

hkllist or numpy array with the Miller indices (or Q(h,k,l) is also possible)

StructureFactor (*q, en='config', temp=0*)

caluclates the structure factor of a material for a certain momentum transfer and energy at a certain temperature of the material

Parameter

qvectorial momentum transfer (vectors as list,tuple or numpy array are valid)

enenergy in eV, if omitted the value from the xrayutilities configuration is used

temptemperature used for Debye-Waller-factor calculation

Returns

the complex structure factor

StructureFactorForEnergy (*q0, en, temp=0*)

caluclates the structure factor of a material for a certain momentum transfer and a bunch of energies

Parameter

q0vectorial momentum transfer (vectors as list,tuple or numpy array are valid)

enlist, tuple or array of energy values in eV

temptemperature used for Debye-Waller-factor calculation

Returns

complex valued structure factor array

StructureFactorForQ (*q, en0='config', temp=0*)

caluclates the structure factor of a material for a bunch of momentum transfers and a certain energy

Parameter

qvectorial momentum transfers; list of vectores (list, tuple or array) of length 3 e.g.:
(Si.Q(0,0,4),Si.Q(0,0,4.1),...) or numpy.array([Si.Q(0,0,4),Si.Q(0,0,4.1)])

en0energy value in eV, if omitted the value from the xrayutilities configuration is used

temptemperature used for Debye-Waller-factor calculation

Returns

complex valued structure factor array

a1

a2

a3

b1

b2**b3****beta** (*en='config'*)

function to calculate the imaginary part of the deviation of the refractive index from 1 ($n=1-\text{delta}+i*\text{beta}$)

Parameter

enx-ray energy eV, if omitted the value from the xrayutilities configuration is used

Returns

beta (float)

chi0 (*en='config'*)

calculates the complex chi_0 values often needed in simulations. They are closely related to delta and beta ($n = 1 + \text{chi_r0}/2 + i*\text{chi_i0}/2$ vs. $n = 1 - \text{delta} + i*\text{beta}$)

chih (*q, en='config', temp=0, polarization='S'*)

calculates the complex polarizability of a material for a certain momentum transfer and energy

Parameter

qmomentum transfer in (1/Å)

enxray energy in eV, if omitted the value from the xrayutilities configuration is used

temptemperature used for Debye-Waller-factor calculation

polarizationeither 'S' (default) sigma or 'P' pi polarization

Returns

(abs(chih_real),abs(chih_imag)) complex polarizability

critical_angle (*en='config', deg=True*)

calculate critical angle for total external reflection

Parameter

enenergy of the x-rays, if omitted the value from the xrayutilities configuration is used

degreturn angle in degree if True otherwise radians (default:True)

Returns

Angle of total external reflection

dTheta (*Q, en='config'*)

function to calculate the refractive peak shift

Parameter

Qmomentum transfer (1/Å)

enx-ray energy (eV), if omitted the value from the xrayutilities configuration is used

Returns

deltaThetapeak shift in degree

delta (*en='config'*)

function to calculate the real part of the deviation of the refractive index from 1 ($n=1-\text{delta}+i*\text{beta}$)

Parameter

enx-ray energy eV, if omitted the value from the xrayutilities configuration is used

Returns

delta (float)

idx_refraction (*en='config'*)

function to calculate the complex index of refraction of a material in the x-ray range

Parameter

enenergy of the x-rays, if omitted the value from the xrayutilities configuration is used

Returns

n (complex)

lam

mu

nu

`xrayutilities.materials.material.PseudomorphicMaterial` (*submat, layermat*)

This function returns a material whos lattice is pseudomorphic on a particular substrate material. This function works meanwhile only for cubic materials.

required input arguments:

submatsubstrate material

layermatbulk material of the layer

return value:An instance of Material holding the new pseudomorphically strained material.

`xrayutilities.materials.material.index_map_ij2ijkl` (*ij*)

`xrayutilities.materials.material.index_map_ijkl2ij` (*i, j*)

predefined_materials Module

class `xrayutilities.materials.predefined_materials.SiGe` (*x*)

Bases: `xrayutilities.materials.material.CubicAlloy`

lattice_const_AB (*latA, latB, x*)

method to calculate the lattice parameter of the SiGe alloy with composition Si_{1-x}Ge_x

x

math Package

math Package

fit Module module with a function wrapper to `scipy.optimize.leastsq` for fitting of a 2D function to a peak or a 1D Gauss fit with the `odr` package

`xrayutilities.math.fit.fit_peak2d` (*x, y, data, start, drange, fit_function, maxfev=2000*)

fit a two dimensional function to a two dimensional data set e.g. a reciprocal space map

Parameters

x,ydata coordinates (do NOT need to be regularly spaced)

datadata set used for fitting (e.g. intensity at the data coords)

startset of starting parameters for the fit used as first parameter of function `fit_function`

drangelimits for the data ranges used in the fitting algorithm e.g. it is clever to use only a small region around the peak which should be fitted: [xmin,xmax,ymin,ymax]

fit_functionfunction which should be fitted must accept the parameters (*x,y,*params*)

Returns

(**fitparam,cov**)the set of fitted parameters and covariance matrix

`xrayutilities.math.fit.gauss_fit (xdata, ydata, iparams=[], maxit=200)`

Gauss fit function using odr-pack wrapper in scipy similar to :https://github.com/tiagopereira/python_tips/wiki/Scipy%3A-curve-fitting

Parameters

xdatacoordinates of the data to be fitted

ydatacoordinates of the data which should be fit

keyword parameters:

iparamsinitial paramters for the fit (determined automatically if nothing is given

maxitmaximal iteration number of the fit

Returns

params,sd_params,itlim

the Gauss parameters as defined in function `Gauss1d(x, *param)` and their errors of the fit, as well as a boolean flag which is false in the case of a successful fit

functions Module module with several common function needed in xray data analysis

`xrayutilities.math.functions.Debye1 (x)`

function to calculate the first Debye function as needed for the calculation of the thermal Debye-Waller-factor by numerical integration

for definition see: :http://en.wikipedia.org/wiki/Debye_function

$D1(x) = (1/x) \int_0^x t/(\exp(t)-1) dt$

Parameters

xargument of the Debye function (float)

Returns

D1(x)float value of the Debye function

`xrayutilities.math.functions.Gauss1d (x, *p)`

function to calculate a general one dimensional Gaussian

Parameters

plist of parameters of the Gaussian [XCEN,SIGMA,AMP,BACKGROUND] for information: $SIGMA = FWHM / (2*\sqrt{2*\log(2)})$

xcoordinate(s) where the function should be evaluated

Returns

the value of the Gaussian described by the parameters p at position x

`xrayutilities.math.functions.Gauss1d_der_p (x, *p)`

function to calculate the derivative of a Gaussian with respect the parameters p

for parameter description see `Gauss1d`

`xrayutilities.math.functions.Gauss1d_der_x (x, *p)`

function to calculate the derivative of a Gaussian with respect to x

for parameter description see `Gauss1d`

`xrayutilities.math.functions.Gauss2d (x, y, *p)`

function to calculate a general two dimensional Gaussian

Parameters

plist of parameters of the Gauss-function [XCEN,YCEN,SIGMAX,SIGMAY,AMP,BACKGROUND,ANGLE]
SIGMA = FWHM / (2*sqrt(2*log(2))) ANGLE = rotation of the X,Y direction of
the Gaussian in radians

x,ycoordinate(s) where the function should be evaluated

Returns

the value of the Gaussian described by the parameters **p** at position (x,y)

`xrayutilities.math.functions.Lorentz1d(x, *p)`
function to calculate a general one dimensional Lorentzian

Parameters

plist of parameters of the Lorentz-function [XCEN,FWHM,AMP,BACKGROUND]

x,ycoordinate(s) where the function should be evaluated

Returns

the value of the Lorentian described by the parameters **p** at position (x,y)

`xrayutilities.math.functions.Lorentz2d(x, y, *p)`
function to calculate a general two dimensional Lorentzian

Parameters

plist of parameters of the Lorentz-function [XCEN,YCEN,FWHMX,FWHMY,AMP,BACKGROUND,ANGLE]
ANGLE = rotation of the X,Y direction of the Lorentzian in radians

x,ycoordinate(s) where the function should be evaluated

Returns

the value of the Lorentian described by the parameters **p** at position (x,y)

`xrayutilities.math.functions.TwoGauss2d(x, y, *p)`
function to calculate two general two dimensional Gaussians

Parameters

plist of parameters of the Gauss-function [XCEN1,YCEN1,SIGMAX1,SIGMAY1,AMP1,ANGLE1,XCEN2,YCEN2,
SIGMA = FWHM / (2*sqrt(2*log(2))) ANGLE = rotation of the X,Y direction of
the Gaussian in radians

x,ycoordinate(s) where the function should be evaluated

Return

the value of the Gaussian described by the parameters **p** at position (x,y)

`xrayutilities.math.functions.kill_spike(data, threshold=2.0)`
function to smooth ****single**** data points which differ from the average of the neighboring data points by
more than the threshold factor. Such spikes will be replaced by the mean value of the next neighbors.

Warning: Use this function carefully not to manipulate your data!

Parameters

data1d numpy array with experimental data

thresholdthreshold factor to identify strange data points

Returns

1d data-array with spikes removed

`xrayutilities.math.functions.smooth(x, n)`
function to smooth an array of data by averaging N adjacent data points

Parameters

x1D data array

nnumber of data points to average

Returns

xsmoothsmoothed array with same length as x

transforms Module

class xrayutilities.math.transforms.**AxisToZ** (*newaxis*)

Bases: xrayutilities.math.transforms.CoordinateTransform

Creates a coordinate transformation to move a certain axis to the z-axis. The rotation is done along the great circle. The x-axis of the new coordinate frame is created to be normal to the new and original z-axis. The new y-axis is create in order to obtain a right handed coordinate system.

xrayutilities.math.transforms.**Cij2Cijkl** (*cij*)

Converts the elastic constants matrix (tensor of rank 2) to the full rank 4 cijkl tensor.

required input arguments:

cij(6,6) cij matrix as a numpy array

return value:

cijkl(3,3,3,3) cijkl tensor as numpy array

xrayutilities.math.transforms.**Cijkl2Cij** (*cijkl*)

Converts the full rank 4 tensor of the elastic constants to the (6,6) matrix of elastic constants.

required input arguments:

cijkl(3,3,3,3) cijkl tensor as numpy array

return value:

cij(6,6) cij matrix as a numpy array

class xrayutilities.math.transforms.**CoordinateTransform** (*v1, v2, v3*)

Bases: xrayutilities.math.transforms.Transform

Create a Transformation object which transforms a point into a new coordinate frame. The new frame is determined by the three vectors v1/norm(v1), v2/norm(v2) and v3/norm(v3), which need to be orthogonal!

class xrayutilities.math.transforms.**Transform** (*matrix*)

Bases: object

inverse (**args*)

performs inverse transformation a vector, matrix or tensor of rank 4

Parameters

***args: object to transform, list or numpy array of shape(n,) (n,n), (n,n,n,n) where n is the rank of the transformation matrix**

xrayutilities.math.transforms.**XRotation** (*alpha, deg=True*)

Returns a transform that represents a rotation about the x-axis by an angle alpha. If deg=True the angle is assumed to be in degree, otherwise the function expects radians.

xrayutilities.math.transforms.**YRotation** (*alpha, deg=True*)

Returns a transform that represents a rotation about the y-axis by an angle alpha. If deg=True the angle is assumed to be in degree, otherwise the function expects radians.

xrayutilities.math.transforms.**ZRotation** (*alpha, deg=True*)

Returns a transform that represents a rotation about the z-axis by an angle alpha. If deg=True the angle is assumed to be in degree, otherwise the function expects radians.

xrayutilities.math.transforms.**index_map_ij2ijkl** (*ij*)

xrayutilities.math.transforms.**index_map_ijkl2ij** (*i, j*)

`xrayutilities.math.transforms.mycross` (*vec, mat*)

function implements the cross-product of a vector with each column of a matrix

`xrayutilities.math.transforms.rotarb` (*vec, axis, ang, deg=True*)

function implements the rotation around an arbitrary axis by an angle *ang* positive rotation is anti-clockwise when looking from positive end of axis vector

Parameter

vec numpy.array or list of length 3

axis numpy.array or list of length 3

ang rotation angle in degree (*deg=True*) or in rad (*deg=False*)

deg boolean which determines the input format of *ang* (default: *True*)

Returns

rotvec rotated vector as numpy.array

Example

```
>>> rotarb([1,0,0],[0,0,1],90)
array([ 6.12323400e-17,  1.00000000e+00,  0.00000000e+00])
```

`xrayutilities.math.transforms.tensorprod` (*vec1, vec2*)

function implements an elementwise multiplication of two vectors

vector Module module with vector operations, mostly numpy functionality is used for the vector operation itself, however custom error checking is done to ensure vectors of length 3.

`xrayutilities.math.vector.VecAngle` (*v1, v2, deg=False*)

calculate the angle between two vectors. The following formula is used $v1.v2 = \text{norm}(v1) * \text{norm}(v2) * \cos(\alpha)$

$\alpha = \arccos((v1.v2)/(\text{norm}(v1) * \text{norm}(v2)))$

required input arguments:

v1 vector as numpy array or list

v2 vector as numpy array or list

optional keyword arguments:

deg (default: *false*) return result in degree otherwise in radians

return value: float value with the angle inclined by the two vectors

`xrayutilities.math.vector.VecDot` (*v1, v2*)

Calculate the vector dot product.

required input arguments:

v1 vector as numpy array or list

v2 vector as numpy array or list

return value: float value

`xrayutilities.math.vector.VecNorm` (*v*)

Calculate the norm of a vector.

required input arguments:

v vector as list or numpy array

return value: float holding the vector norm

`xrayutilities.math.vector.VecUnit` (*v*)

Calculate the unit vector of *v*.

required input arguments:

vvector as list or numpy array

return value: numpy array with the unit vector

`xrayutilities.math.vector.getSyntax` (*vec*)

returns vector direction in the syntax 'x+' 'z-' or equivalents therefore works only for principle vectors of the coordinate system like e.g. [1,0,0] or [0,2,0]

Parameters

string[xyz][+-]

Returns

vector along the given direction as numpy array

`xrayutilities.math.vector.getVector` (*string*)

returns unit vector along a rotation axis given in the syntax 'x+' 'z-' or equivalents

Parameters

string[xyz][+-]

Returns

vector along the given direction as numpy array

INDICES AND TABLES

- *genindex*
- *modindex*
- *search*

PYTHON MODULE INDEX

X

xrayutilities, 9
xrayutilities.__init__, 110
xrayutilities.analysis, 124
xrayutilities.analysis.line_cuts, 124
xrayutilities.analysis.line_cuts3d, 131
xrayutilities.analysis.misc, 132
xrayutilities.analysis.sample_align, 132
xrayutilities.config, 110
xrayutilities.exception, 110
xrayutilities.experiment, 110
xrayutilities.gridder, 120
xrayutilities.gridder2d, 120
xrayutilities.gridder3d, 121
xrayutilities.io, 136
xrayutilities.io.edf, 137
xrayutilities.io.imagereader, 137
xrayutilities.io.panalytical_xml, 138
xrayutilities.io.radicon, 138
xrayutilities.io.rotanode_alignment, 139
xrayutilities.io.seifert, 139
xrayutilities.io.spec, 141
xrayutilities.io.spectra, 143
xrayutilities.materials, 146
xrayutilities.materials._create_database, 146
xrayutilities.materials._create_database_alt, 146
xrayutilities.materials.cif, 146
xrayutilities.materials.database, 146
xrayutilities.materials.elements, 148
xrayutilities.materials.lattice, 148
xrayutilities.materials.material, 150
xrayutilities.materials.predefined_materials, 154
xrayutilities.math, 154
xrayutilities.math.fit, 154
xrayutilities.math.functions, 155
xrayutilities.math.transforms, 157
xrayutilities.math.vector, 158
xrayutilities.normalize, 121
xrayutilities.utilities, 123

xrayutilities.utilities_noconf, 123

INDEX

A

a1 (xrayutilities.materials.material.Material attribute), 67, 103, 152
a2 (xrayutilities.materials.material.Material attribute), 67, 103, 152
a3 (xrayutilities.materials.material.Material attribute), 67, 103, 152
abs_corr() (xrayutilities.io.spectra.Spectra method), 58, 94, 144
absfun (xrayutilities.normalize.IntensityNormalizer attribute), 35, 121
add_f0_from_intertab() (in module xrayutilities.materials.database), 62, 98, 147
add_f0_from_xop() (in module xrayutilities.materials.database), 62, 98, 147
add_f1f2_from_ascii_file() (in module xrayutilities.materials.database), 62, 98, 148
add_f1f2_from_henkedb() (in module xrayutilities.materials.database), 62, 98, 148
add_f1f2_from_kissel() (in module xrayutilities.materials.database), 62, 98, 148
add_mass_from_NIST() (in module xrayutilities.materials.database), 62, 98, 148
Alloy (class in xrayutilities.materials.material), 64, 100, 150
Ang2HKL() (xrayutilities.experiment.Experiment method), 24, 110
Ang2Q() (xrayutilities.experiment.GID method), 25, 111
Ang2Q() (xrayutilities.experiment.GID_ID10B method), 26, 112
Ang2Q() (xrayutilities.experiment.GISAXS method), 27, 113
Ang2Q() (xrayutilities.experiment.HXRD method), 28, 114
Ang2Q() (xrayutilities.experiment.NonCOP method), 29, 115
append() (xrayutilities.io.spectra.SPECTRAFileData method), 58, 94, 144
append() (xrayutilities.materials.lattice.LatticeBase method), 64, 100, 149
ApplyStrain() (xrayutilities.materials.lattice.Lattice method), 63, 99, 149
ApplyStrain() (xrayutilities.materials.material.Material method), 66, 102, 152

area() (xrayutilities.experiment.QCConversion method), 30, 116
area_detector_calib() (in module xrayutilities.analysis.sample_align), 46, 82, 132
area_detector_calib_hkl() (in module xrayutilities.analysis.sample_align), 47, 83, 133
Atom (class in xrayutilities.materials.lattice), 62, 98, 148
avmon (xrayutilities.normalize.IntensityNormalizer attribute), 35, 121
axis() (in module xrayutilities.gridder), 34, 120
AxisToZ (class in xrayutilities.math.transforms), 71, 107, 157

B

B (xrayutilities.materials.material.Material attribute), 66, 102, 152
b1 (xrayutilities.materials.material.Material attribute), 67, 103, 152
b2 (xrayutilities.materials.material.Material attribute), 67, 103, 152
b3 (xrayutilities.materials.material.Material attribute), 67, 103, 153
BaddeleyiteLattice() (in module xrayutilities.materials.lattice), 63, 99, 148
BCCLattice() (in module xrayutilities.materials.lattice), 63, 99, 148
BCTLattice() (in module xrayutilities.materials.lattice), 63, 99, 148
beta() (xrayutilities.materials.material.Material method), 67, 103, 153
blockAverage1D() (in module xrayutilities.normalize), 36, 122
blockAverage2D() (in module xrayutilities.normalize), 36, 122
blockAveragePSD() (in module xrayutilities.normalize), 36, 122

C

check_array() (in module xrayutilities.gridder), 34, 120
chi0() (xrayutilities.materials.material.Material method), 67, 103, 153
chih() (xrayutilities.materials.material.Material method), 67, 103, 153
CIFFFile (class in xrayutilities.materials.cif), 60, 96, 146

Cij2Cijkl() (in module xrayutilities.materials.material), 65, 101, 150
Cij2Cijkl() (in module xrayutilities.math.transforms), 71, 107, 157
Cijkl2Cij() (in module xrayutilities.materials.material), 65, 101, 150
Cijkl2Cij() (in module xrayutilities.math.transforms), 72, 108, 157
Clear() (xrayutilities.gridder.Gridder1D method), 34, 120
Clear() (xrayutilities.gridder2d.Gridder2D method), 34, 120
ClearData() (xrayutilities.io.spec.SPECSScan method), 56, 92, 142
Close() (xrayutilities.materials.database.DataBase method), 61, 97, 146
ContentBasym() (xrayutilities.materials.material.CubicAlloy method), 65, 101, 150
ContentBsym() (xrayutilities.materials.material.CubicAlloy method), 65, 101, 151
Convolute() (xrayutilities.experiment.Powder method), 30, 116
CoordinateTransform (class in xrayutilities.math.transforms), 72, 108, 157
Create() (xrayutilities.materials.database.DataBase method), 61, 97, 146
CreateMaterial() (xrayutilities.materials.database.DataBase method), 61, 97, 146
critical_angle() (xrayutilities.materials.material.Material method), 68, 104, 153
CubicAlloy (class in xrayutilities.materials.material), 65, 101, 150
CubicElasticTensor() (in module xrayutilities.materials.material), 65, 101, 151
CubicFm3mBaF2() (in module xrayutilities.materials.lattice), 63, 99, 148
CubicLattice() (in module xrayutilities.materials.lattice), 63, 99, 148
CuMnAsLattice() (in module xrayutilities.materials.lattice), 63, 99, 148

D

darkfield (xrayutilities.normalize.IntensityNormalizer attribute), 35, 121
data (xrayutilities.gridder.Gridder1D attribute), 34, 120
data (xrayutilities.gridder2d.Gridder2D attribute), 34, 121
DataBase (class in xrayutilities.materials.database), 61, 97, 146
Debye1() (in module xrayutilities.math.functions), 70, 106, 155
delta() (in module xrayutilities.gridder), 34, 120
delta() (xrayutilities.materials.material.Material method), 68, 104, 153

det (xrayutilities.normalize.IntensityNormalizer attribute), 35, 121
detectorAxis (xrayutilities.experiment.QConversion attribute), 31, 117
DiamondLattice() (in module xrayutilities.materials.lattice), 63, 99, 148
dTheta() (xrayutilities.materials.material.Material method), 68, 104, 153
dump2h5() (xrayutilities.io.seifert.SeifertScan method), 54, 90, 140
dump2hdf5() (xrayutilities.io.seifert.SeifertMultiScan method), 54, 90, 139
dump2mlab() (xrayutilities.io.seifert.SeifertMultiScan method), 54, 90, 140
dump2mlab() (xrayutilities.io.seifert.SeifertScan method), 54, 90, 140

E

EDFDirectory (class in xrayutilities.io.edf), 51, 87, 137
EDFFile (class in xrayutilities.io.edf), 51, 87, 137
energy (xrayutilities.experiment.Experiment attribute), 25, 111
energy (xrayutilities.experiment.QConversion attribute), 31, 117
energy() (in module xrayutilities.utilities_noconf), 37, 123
Experiment (class in xrayutilities.experiment), 24, 110

F

f() (xrayutilities.materials.lattice.Atom method), 62, 98, 148
f0() (xrayutilities.materials.lattice.Atom method), 63, 99, 148
f1() (xrayutilities.materials.lattice.Atom method), 63, 99, 148
f2() (xrayutilities.materials.lattice.Atom method), 63, 99, 148
FCCLLattice() (in module xrayutilities.materials.lattice), 63, 99, 148
fit_bragg_peak() (in module xrayutilities.analysis.sample_align), 48, 84, 134
fit_peak2d() (in module xrayutilities.math.fit), 69, 105, 154
flatfield (xrayutilities.normalize.IntensityNormalizer attribute), 35, 122
fwhm_exp() (in module xrayutilities.analysis.line_cuts), 38, 74, 124

G

Gauss1d() (in module xrayutilities.math.functions), 70, 106, 155
Gauss1d_der_p() (in module xrayutilities.math.functions), 70, 106, 155
Gauss1d_der_x() (in module xrayutilities.math.functions), 70, 106, 155
Gauss2d() (in module xrayutilities.math.functions), 70, 106, 155

- gauss_fit() (in module xrayutilities.math.fit), 69, 105, 155
- GeneralPrimitiveLattice() (in module xrayutilities.materials.lattice), 63, 99, 148
- GeneralUC() (in module xrayutilities.materials.material), 66, 102, 151
- get() (xrayutilities.io.rotanode_alignment.RA_Alignment method), 53, 89, 139
- get_omega_scan_ang() (in module xrayutilities.analysis.line_cuts), 38, 74, 124
- get_omega_scan_bounds_ang() (in module xrayutilities.analysis.line_cuts), 39, 75, 125
- get_omega_scan_q() (in module xrayutilities.analysis.line_cuts), 39, 75, 125
- get_qx_scan() (in module xrayutilities.analysis.line_cuts), 40, 76, 126
- get_qx_scan3d() (in module xrayutilities.analysis.line_cuts3d), 45, 81, 131
- get_qy_scan3d() (in module xrayutilities.analysis.line_cuts3d), 45, 81, 131
- get_qz_scan() (in module xrayutilities.analysis.line_cuts), 40, 76, 126
- get_qz_scan3d() (in module xrayutilities.analysis.line_cuts3d), 45, 81, 131
- get_qz_scan_int() (in module xrayutilities.analysis.line_cuts), 40, 77, 127
- get_radial_scan_ang() (in module xrayutilities.analysis.line_cuts), 41, 77, 127
- get_radial_scan_bounds_ang() (in module xrayutilities.analysis.line_cuts), 42, 78, 128
- get_radial_scan_q() (in module xrayutilities.analysis.line_cuts), 42, 78, 128
- get_spectra_files() (in module xrayutilities.io.spectra), 59, 95, 145
- get_ttheta_scan_ang() (in module xrayutilities.analysis.line_cuts), 43, 79, 129
- get_ttheta_scan_bounds_ang() (in module xrayutilities.analysis.line_cuts), 43, 79, 129
- get_ttheta_scan_q() (in module xrayutilities.analysis.line_cuts), 44, 80, 130
- getangles() (in module xrayutilities.analysis.misc), 46, 82, 132
- GetF0() (xrayutilities.materials.database.DataBase method), 61, 97, 147
- GetF1() (xrayutilities.materials.database.DataBase method), 61, 97, 147
- GetF2() (xrayutilities.materials.database.DataBase method), 61, 97, 147
- geth5_scan() (in module xrayutilities.io.spec), 57, 93, 142
- geth5_spectra_map() (in module xrayutilities.io.spectra), 59, 95, 145
- getindex() (in module xrayutilities.analysis.line_cuts), 44, 80, 130
- getindex3d() (in module xrayutilities.analysis.line_cuts3d), 46, 82, 132
- GetMismatch() (xrayutilities.materials.material.Material method), 66, 102, 152
- getOmPixel() (in module xrayutilities.io.panalytical_xml), 52, 88, 138
- GetPoint() (xrayutilities.materials.lattice.Lattice method), 63, 99, 149
- getSeifert_map() (in module xrayutilities.io.seifert), 54, 90, 140
- getSyntax() (in module xrayutilities.math.vector), 73, 109, 159
- getVector() (in module xrayutilities.math.vector), 73, 109, 159
- getxrml_map() (in module xrayutilities.io.panalytical_xml), 52, 88, 138
- GID (class in xrayutilities.experiment), 25, 111
- GID_ID10B (class in xrayutilities.experiment), 26, 112
- GISAXS (class in xrayutilities.experiment), 27, 113
- Gridder (class in xrayutilities.gridder), 34, 120
- Gridder1D (class in xrayutilities.gridder), 34, 120
- Gridder2D (class in xrayutilities.gridder2d), 34, 120
- Gridder3D (class in xrayutilities.gridder3d), 35, 121
- ## H
- HCPLattice() (in module xrayutilities.materials.lattice), 63, 99, 148
- Hexagonal3CLattice() (in module xrayutilities.materials.lattice), 63, 99, 149
- Hexagonal4HLattice() (in module xrayutilities.materials.lattice), 63, 99, 149
- Hexagonal6HLattice() (in module xrayutilities.materials.lattice), 63, 99, 149
- HexagonalElasticTensor() (in module xrayutilities.materials.material), 66, 102, 151
- hst2hdf5() (in module xrayutilities.io.radicon), 52, 88, 138
- HXRD (class in xrayutilities.experiment), 27, 114
- ## I
- idx_refraction() (xrayutilities.materials.material.Material method), 68, 104, 153
- ImageReader (class in xrayutilities.io.imagereader), 51, 87, 137
- index_map_ij2ijkl() (in module xrayutilities.materials.material), 68, 104, 154
- index_map_ij2ijkl() (in module xrayutilities.math.transforms), 72, 108, 157
- index_map_ijkl2ij() (in module xrayutilities.materials.material), 68, 104, 154
- index_map_ijkl2ij() (in module xrayutilities.math.transforms), 72, 108, 157
- init_area() (xrayutilities.experiment.QConversion method), 31, 117
- init_linear() (xrayutilities.experiment.QConversion method), 32, 118
- init_material_db() (in module xrayutilities.materials.database), 62, 98, 148
- InputError, 24, 110

IntensityNormalizer (class in xrayutilities.normalize), 35, 121
inverse() (xrayutilities.math.transforms.Transform method), 72, 108, 157

K

KeepData() (xrayutilities.gridder.Gridder method), 34, 120
keys() (xrayutilities.io.rotanode_alignment.RA_Alignment method), 53, 89, 139
kill_spike() (in module xrayutilities.math.functions), 71, 107, 156

L

lam (xrayutilities.materials.material.Material attribute), 68, 104, 154
lam2en() (in module xrayutilities.utilities_noconf), 37, 123
Lattice (class in xrayutilities.materials.lattice), 63, 99, 149
Lattice() (xrayutilities.materials.cif.CIFFile method), 60, 96, 146
lattice_const_AB() (xrayutilities.materials.material.Alloy method), 64, 100, 150
lattice_const_AB() (xrayutilities.materials.predefined_materials.SiGe method), 69, 105, 154
LatticeBase (class in xrayutilities.materials.lattice), 64, 100, 149
linear() (xrayutilities.experiment.QConversion method), 32, 118
linear_detector_calib() (in module xrayutilities.analysis.sample_align), 48, 84, 134
Lorentz1d() (in module xrayutilities.math.functions), 70, 106, 156
Lorentz2d() (in module xrayutilities.math.functions), 70, 106, 156

M

maplog() (in module xrayutilities.utilities), 36, 123
Material (class in xrayutilities.materials.material), 66, 102, 151
miscut_calc() (in module xrayutilities.analysis.sample_align), 49, 85, 135
mon (xrayutilities.normalize.IntensityNormalizer attribute), 35, 122
mu (xrayutilities.materials.material.Material attribute), 68, 104, 154
mycross() (in module xrayutilities.math.transforms), 72, 108, 157

N

NaumanniteLattice() (in module xrayutilities.materials.lattice), 64, 100, 149
NonCOP (class in xrayutilities.experiment), 29, 115
Normalize() (xrayutilities.gridder.Gridder method), 34, 120

nu (xrayutilities.materials.material.Material attribute), 68, 104, 154

O

ones() (in module xrayutilities.gridder), 34, 120
Open() (xrayutilities.materials.database.DataBase method), 61, 97, 147

P

Parse() (xrayutilities.io.rotanode_alignment.RA_Alignment method), 53, 89, 139
parse() (xrayutilities.io.seifert.SeifertMultiScan method), 54, 90, 140
parse() (xrayutilities.io.seifert.SeifertScan method), 54, 90, 140
Parse() (xrayutilities.io.spec.SPECFFile method), 55, 91, 141
Parse() (xrayutilities.io.spec.SPECLog method), 56, 92, 141
Parse() (xrayutilities.materials.cif.CIFFile method), 61, 97, 146
PerkinElmer (class in xrayutilities.io.imagereader), 51, 87, 137
PerovskiteTypeRhombohedral() (in module xrayutilities.materials.lattice), 64, 100, 149
plot() (xrayutilities.io.rotanode_alignment.RA_Alignment method), 53, 89, 139
plot() (xrayutilities.io.spec.SPECSScan method), 57, 93, 142
point() (xrayutilities.experiment.QConversion method), 33, 119
Powder (class in xrayutilities.experiment), 30, 116
PowderIntensity() (xrayutilities.experiment.Powder method), 30, 116
psd_chdeg() (in module xrayutilities.analysis.sample_align), 49, 85, 135
psd_refl_align() (in module xrayutilities.analysis.sample_align), 50, 86, 136
PseudomorphicMaterial() (in module xrayutilities.materials.material), 68, 104, 154

Q

Q() (xrayutilities.materials.material.Material method), 66, 102, 152
Q2Ang() (xrayutilities.experiment.Experiment method), 25, 111
Q2Ang() (xrayutilities.experiment.GID method), 26, 112
Q2Ang() (xrayutilities.experiment.GID_ID10B method), 26, 113
Q2Ang() (xrayutilities.experiment.GISAXS method), 27, 114
Q2Ang() (xrayutilities.experiment.HXRD method), 28, 114
Q2Ang() (xrayutilities.experiment.NonCOP method), 29, 116
Q2Ang() (xrayutilities.experiment.Powder method), 30, 116

QConversion (class in xrayutilities.experiment), 30, 116

QuartzLattice() (in module xrayutilities.materials.lattice), 64, 100, 149

R

RA_Alignment (class in xrayutilities.io.rotanode_alignment), 53, 89, 139

rad2hdf5() (in module xrayutilities.io.radicon), 53, 89, 138

Read() (xrayutilities.io.spectra.SPECTRAFile method), 58, 94, 143

read_data() (in module xrayutilities.io.spectra), 60, 96, 145

read_mca() (in module xrayutilities.io.spectra), 60, 96, 145

read_mca_dir() (in module xrayutilities.io.spectra), 60, 96, 146

read_mcas() (in module xrayutilities.io.spectra), 60, 96, 146

ReadData() (xrayutilities.io.edf.EDFFile method), 51, 87, 137

ReadData() (xrayutilities.io.spec.SPECMCAFile method), 56, 92, 141

ReadData() (xrayutilities.io.spec.SPECMCAInline method), 56, 92, 142

ReadData() (xrayutilities.io.spec.SPECSScan method), 56, 92, 142

readImage() (xrayutilities.io.imagereader.ImageReader method), 51, 87, 137

ReadMCA() (xrayutilities.io.spectra.SPECTRAFile method), 58, 94, 143

recarray2hdf5() (xrayutilities.io.spectra.Spectra method), 59, 95, 144

ReciprocalLattice() (xrayutilities.materials.lattice.Lattice method), 63, 99, 149

RelaxationTriangle() (xrayutilities.materials.material.Alloy method), 64, 100, 150

repair_key() (in module xrayutilities.io.seifert), 55, 91, 141

RockSalt_Cubic_Lattice() (in module xrayutilities.materials.lattice), 64, 100, 149

RockSaltLattice() (in module xrayutilities.materials.lattice), 64, 100, 149

RoperCCD (class in xrayutilities.io.imagereader), 52, 88, 137

rotarb() (in module xrayutilities.math.transforms), 72, 108, 158

RutileLattice() (in module xrayutilities.materials.lattice), 64, 100, 149

S

sampleAxis (xrayutilities.experiment.QConversion attribute), 33, 119

Save2HDF5() (xrayutilities.io.edf.EDFDirectory method), 51, 87, 137

Save2HDF5() (xrayutilities.io.edf.EDFFile method), 51, 87, 137

Save2HDF5() (xrayutilities.io.spec.SPECCmdLine method), 55, 91, 141

Save2HDF5() (xrayutilities.io.spec.SPECFile method), 55, 91, 141

Save2HDF5() (xrayutilities.io.spec.SPECSScan method), 56, 92, 142

Save2HDF5() (xrayutilities.io.spectra.SPECTRAFile method), 58, 94, 143

save_h5_attrs() (xrayutilities.io.seifert.SeifertHeader method), 54, 90, 139

SeifertHeader (class in xrayutilities.io.seifert), 54, 90, 139

SeifertMultiScan (class in xrayutilities.io.seifert), 54, 90, 139

SeifertScan (class in xrayutilities.io.seifert), 54, 90, 140

selecthst() (in module xrayutilities.io.radicon), 53, 89, 139

set_abs_factors() (xrayutilities.io.spectra.Spectra method), 59, 95, 144

SetF0() (xrayutilities.materials.database.DataBase method), 61, 97, 147

SetF1() (xrayutilities.materials.database.DataBase method), 62, 97, 147

SetF2() (xrayutilities.materials.database.DataBase method), 62, 98, 147

SetMaterial() (xrayutilities.materials.database.DataBase method), 62, 98, 147

SetMCAParams() (xrayutilities.io.spec.SPECSScan method), 56, 92, 142

SetResolution() (xrayutilities.gridder2d.Gridder2D method), 34, 121

SetResolution() (xrayutilities.gridder3d.Gridder3D method), 35, 121

SetWeight() (xrayutilities.materials.database.DataBase method), 62, 98, 147

SiGe (class in xrayutilities.materials.predefined_materials), 69, 105, 154

smooth() (in module xrayutilities.math.functions), 71, 107, 156

SPECCmdLine (class in xrayutilities.io.spec), 55, 91, 141

SPECFile (class in xrayutilities.io.spec), 55, 91, 141

SPECLog (class in xrayutilities.io.spec), 56, 92, 141

SPECMCA (class in xrayutilities.io.spec), 56, 92, 141

SPECMCAFile (class in xrayutilities.io.spec), 56, 92, 141

SPECMCAInline (class in xrayutilities.io.spec), 56, 92, 141

SPECSScan (class in xrayutilities.io.spec), 56, 92, 142

Spectra (class in xrayutilities.io.spectra), 58, 94, 144

spectra2hdf5() (xrayutilities.io.spectra.Spectra method), 59, 95, 144

SPECTRAFile (class in xrayutilities.io.spectra), 57, 93, 143

SPECTRAFileComments (class in xrayutilities.io.spectra), 58, 94, 144
SPECTRAFileData (class in xrayutilities.io.spectra), 58, 94, 144
SPECTRAFileDataColumn (class in xrayutilities.io.spectra), 58, 94, 144
SPECTRAFileParameters (class in xrayutilities.io.spectra), 58, 94, 144
StructureFactor() (xrayutilities.materials.material.Material method), 66, 102, 152
StructureFactorForEnergy() (xrayutilities.materials.material.Material method), 67, 103, 152
StructureFactorForQ() (xrayutilities.materials.material.Material method), 67, 103, 152
SymStruct() (xrayutilities.materials.cif.CIFFile method), 61, 97, 146

T

tensorprod() (in module xrayutilities.math.transforms), 73, 109, 158
TetragonalIndiumLattice() (in module xrayutilities.materials.lattice), 64, 100, 149
TetragonalTinLattice() (in module xrayutilities.materials.lattice), 64, 100, 149
TiltAngle() (xrayutilities.experiment.Experiment method), 25, 111
time (xrayutilities.normalize.IntensityNormalizer attribute), 35, 122
Transform (class in xrayutilities.math.transforms), 72, 108, 157
Transform() (xrayutilities.experiment.Experiment method), 25, 111
TrigonalR3mh() (in module xrayutilities.materials.lattice), 64, 100, 150
TwoGauss2d() (in module xrayutilities.math.functions), 71, 107, 156

U

UB (xrayutilities.experiment.QConversion attribute), 30, 116
UnitCellVolume() (xrayutilities.materials.lattice.Lattice method), 64, 100, 149
Update() (xrayutilities.io.spec.SPECFFile method), 56, 92, 141
Update() (xrayutilities.io.spec.SPECLog method), 56, 92, 141

V

VecAngle() (in module xrayutilities.math.vector), 73, 109, 158
VecDot() (in module xrayutilities.math.vector), 73, 109, 158
VecNorm() (in module xrayutilities.math.vector), 73, 109, 158

VecUnit() (in module xrayutilities.math.vector), 73, 109, 158

W

wavelength (xrayutilities.experiment.Experiment attribute), 25, 111
wavelength (xrayutilities.experiment.QConversion attribute), 33, 120
wavelength() (in module xrayutilities.utilities_noconf), 37, 123
WurtziteLattice() (in module xrayutilities.materials.lattice), 64, 100, 150

X

x (xrayutilities.materials.material.Alloy attribute), 65, 100, 150
x (xrayutilities.materials.predefined_materials.SiGe attribute), 69, 105, 154
xaxis (xrayutilities.gridder.Gridder1D attribute), 34, 120
xaxis (xrayutilities.gridder2d.Gridder2D attribute), 35, 121
xaxis (xrayutilities.gridder3d.Gridder3D attribute), 35, 121
xmatrix (xrayutilities.gridder2d.Gridder2D attribute), 35, 121
xmatrix (xrayutilities.gridder3d.Gridder3D attribute), 35, 121
xrayutilities (module), 9
xrayutilities.__init__ (module), 24, 110
xrayutilities.analysis (module), 38, 74, 124
xrayutilities.analysis.line_cuts (module), 38, 74, 124
xrayutilities.analysis.line_cuts3d (module), 45, 81, 131
xrayutilities.analysis.misc (module), 46, 82, 132
xrayutilities.analysis.sample_align (module), 46, 82, 132
xrayutilities.config (module), 24, 110
xrayutilities.exception (module), 24, 110
xrayutilities.experiment (module), 24, 110
xrayutilities.gridder (module), 34, 120
xrayutilities.gridder2d (module), 34, 120
xrayutilities.gridder3d (module), 35, 121
xrayutilities.io (module), 51, 87, 136
xrayutilities.io.edf (module), 51, 87, 137
xrayutilities.io.imagereader (module), 51, 87, 137
xrayutilities.io.panalytical_xml (module), 52, 88, 138
xrayutilities.io.radicon (module), 52, 88, 138
xrayutilities.io.rotanode_alignment (module), 53, 89, 139
xrayutilities.io.seifert (module), 54, 90, 139
xrayutilities.io.spec (module), 55, 91, 141
xrayutilities.io.spectra (module), 57, 93, 143
xrayutilities.materials (module), 60, 96, 146
xrayutilities.materials._create_database (module), 60, 96, 146
xrayutilities.materials._create_database_alt (module), 60, 96, 146
xrayutilities.materials.cif (module), 60, 96, 146

xrayutilities.materials.database (module), 61, 97, 146
xrayutilities.materials.elements (module), 62, 98, 148
xrayutilities.materials.lattice (module), 62, 98, 148
xrayutilities.materials.material (module), 64, 100, 150
xrayutilities.materials.predefined_materials (module),
69, 105, 154
xrayutilities.math (module), 69, 105, 154
xrayutilities.math.fit (module), 69, 105, 154
xrayutilities.math.functions (module), 70, 106, 155
xrayutilities.math.transforms (module), 71, 107, 157
xrayutilities.math.vector (module), 73, 109, 158
xrayutilities.normalize (module), 35, 121
xrayutilities.utilities (module), 36, 123
xrayutilities.utilities_noconf (module), 37, 123
XRDMLEFile (class in xrayutilities.io.panalytical_xml),
52, 88, 138
XRDMLEMeasurement (class in xrayutilities.io.panalytical_xml), 52, 88, 138
XRotation() (in module xrayutilities.math.transforms),
72, 108, 157

Y

yaxis (xrayutilities.gridder2d.Gridder2D attribute), 35,
121
yaxis (xrayutilities.gridder3d.Gridder3D attribute), 35,
121
ymatrix (xrayutilities.gridder2d.Gridder2D attribute),
35, 121
ymatrix (xrayutilities.gridder3d.Gridder3D attribute),
35, 121
YRotation() (in module xrayutilities.math.transforms),
72, 108, 157

Z

zaxis (xrayutilities.gridder3d.Gridder3D attribute), 35,
121
ZincBlendeLattice() (in module xrayutilities.materials.lattice), 64, 100, 150
zmatrix (xrayutilities.gridder3d.Gridder3D attribute),
35, 121
ZRotation() (in module xrayutilities.math.transforms),
72, 108, 157